

# Artificial Intelligence in Engineering and Sciences

by  
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University of Reading

at  
University of Surrey  
06 December 2022

# Agenda

**1. What are the AI Tools?**

(scope)

**2. What problems do they solve?**

(domain)

**3. How do they solve problems?**

(algorithms)

# What we want to know

**1. to understand the data**

(data collection, processing, and modelling)

**2. to make some prediction**

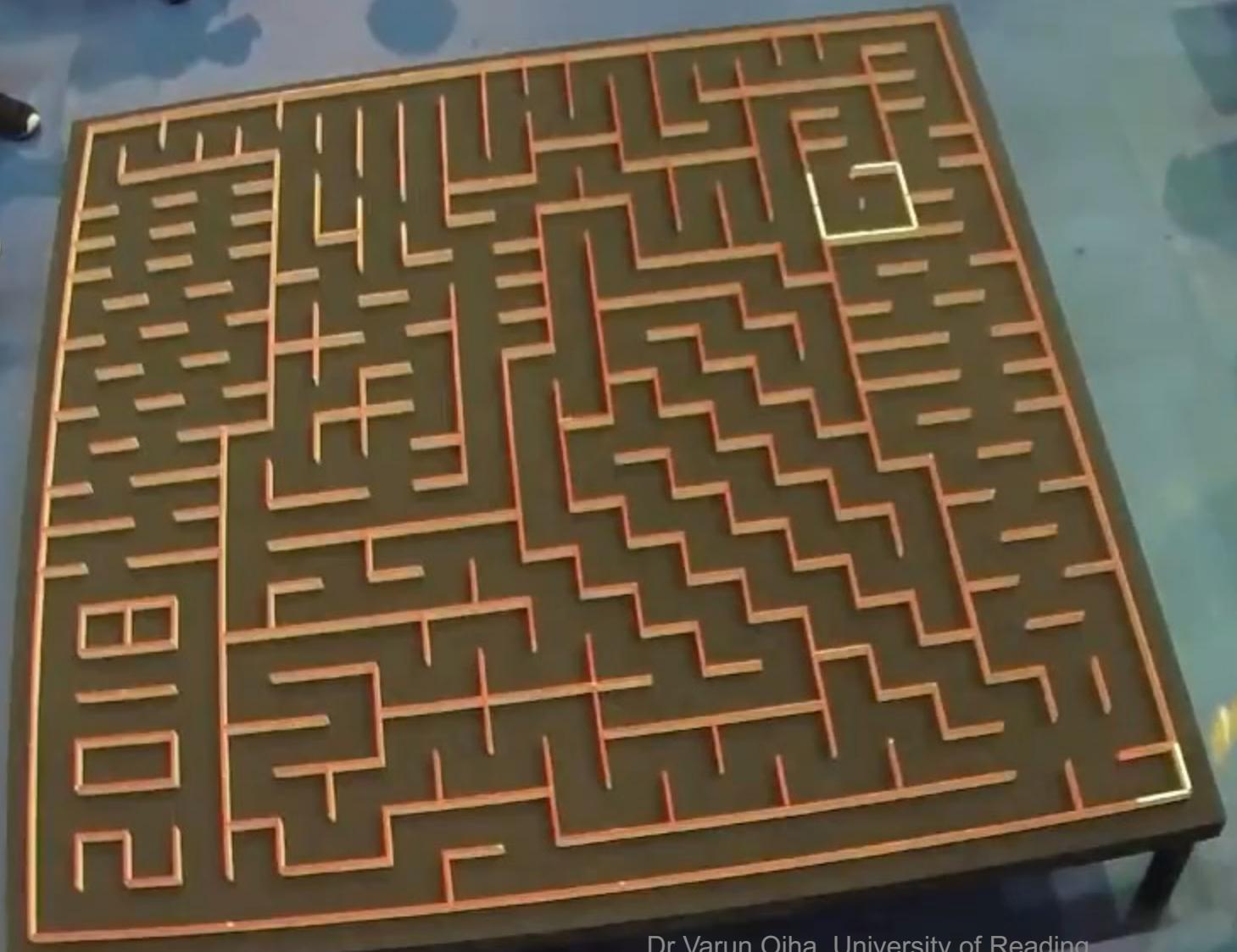
(forecasting)

**3. to optimize some systems**

(discovering appropriate parameters, variables, and settings)

# Artificial Intelligence

to create intelligent machines that  
**think** (react) and **act** (work) like  
human beings

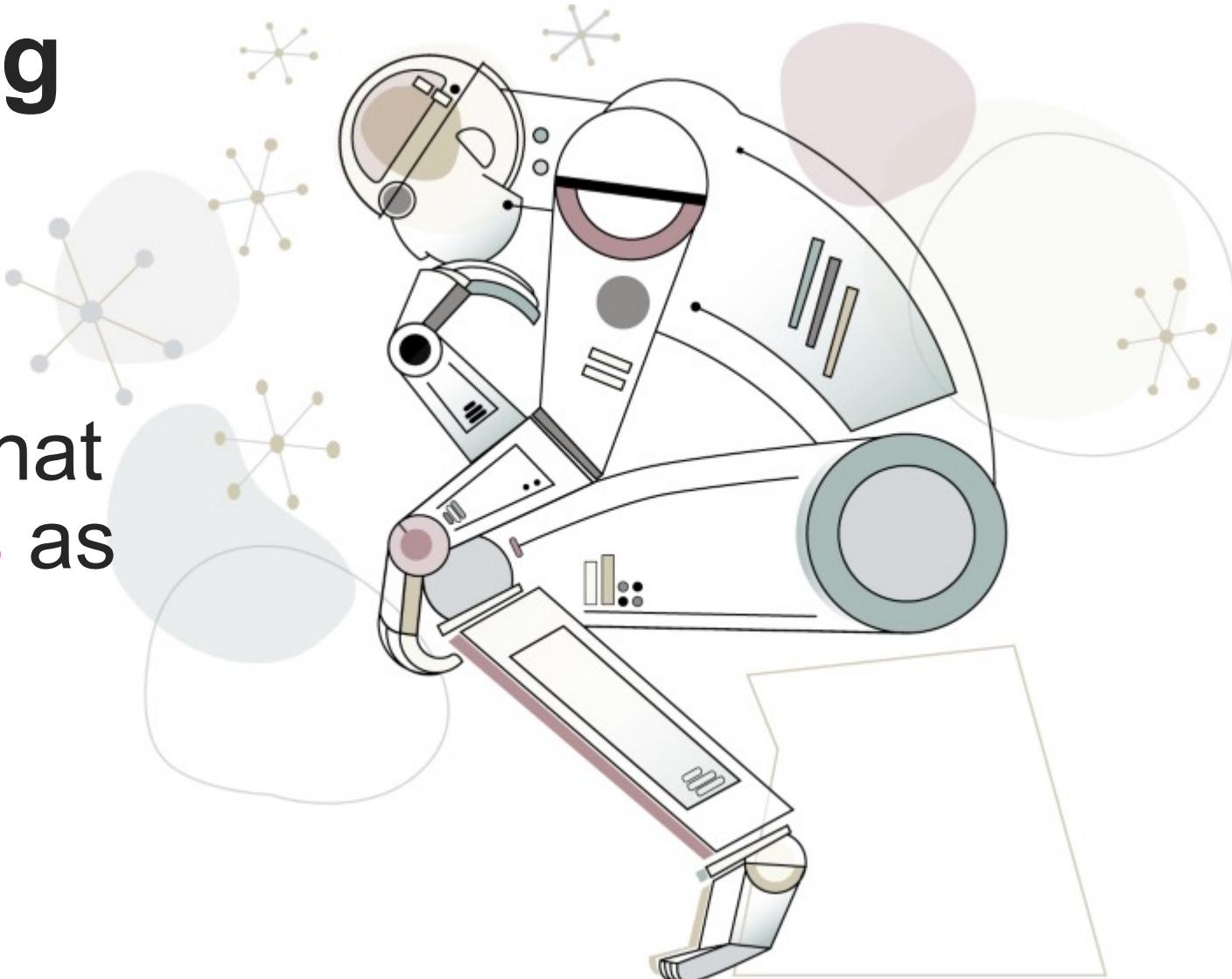


Dr Varun Ojha, University of Reading



# Machine Learning

to create **machines** that  
**learn from examples** as  
living beings do



# Learning

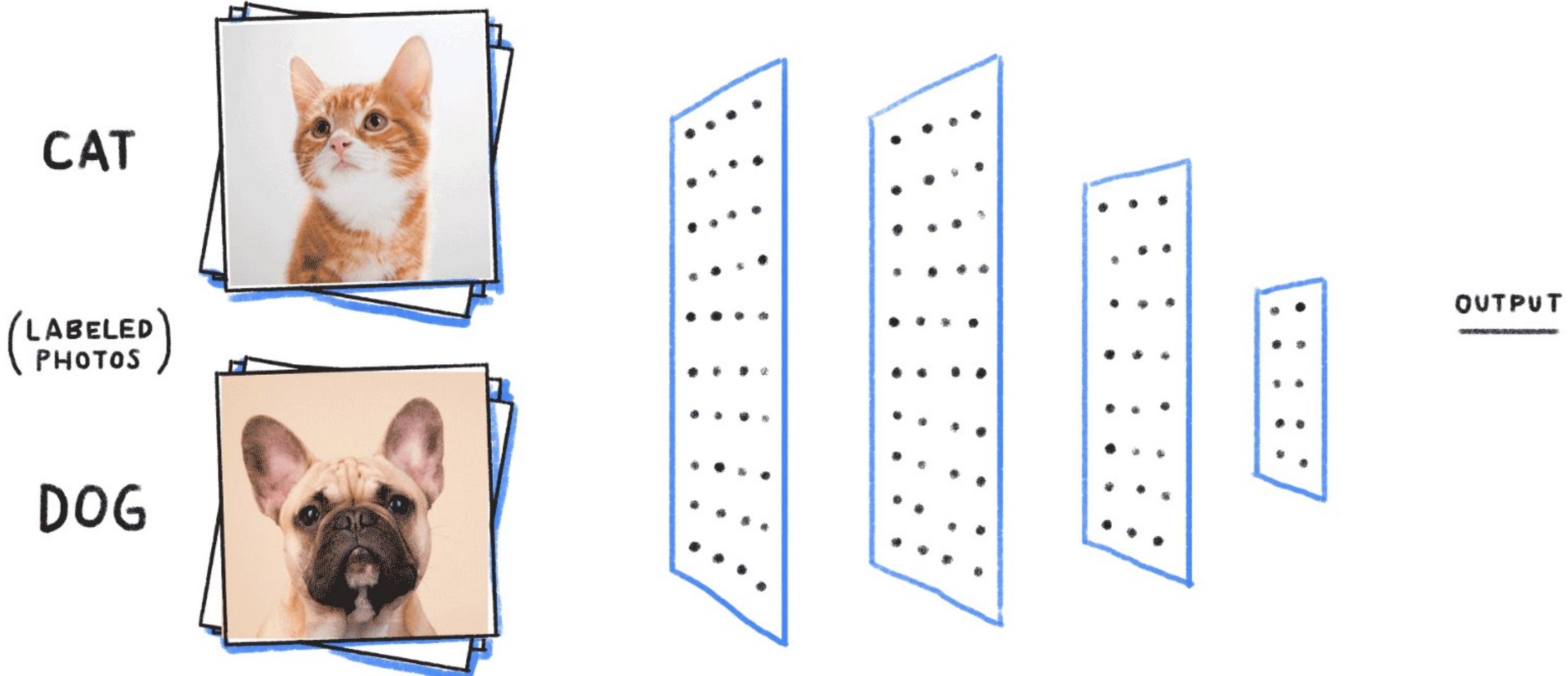
Video Source:

<https://www.youtube.com/watch?v=Ak7bPuR2rDw>  
(Accessed on 21 February 2021)



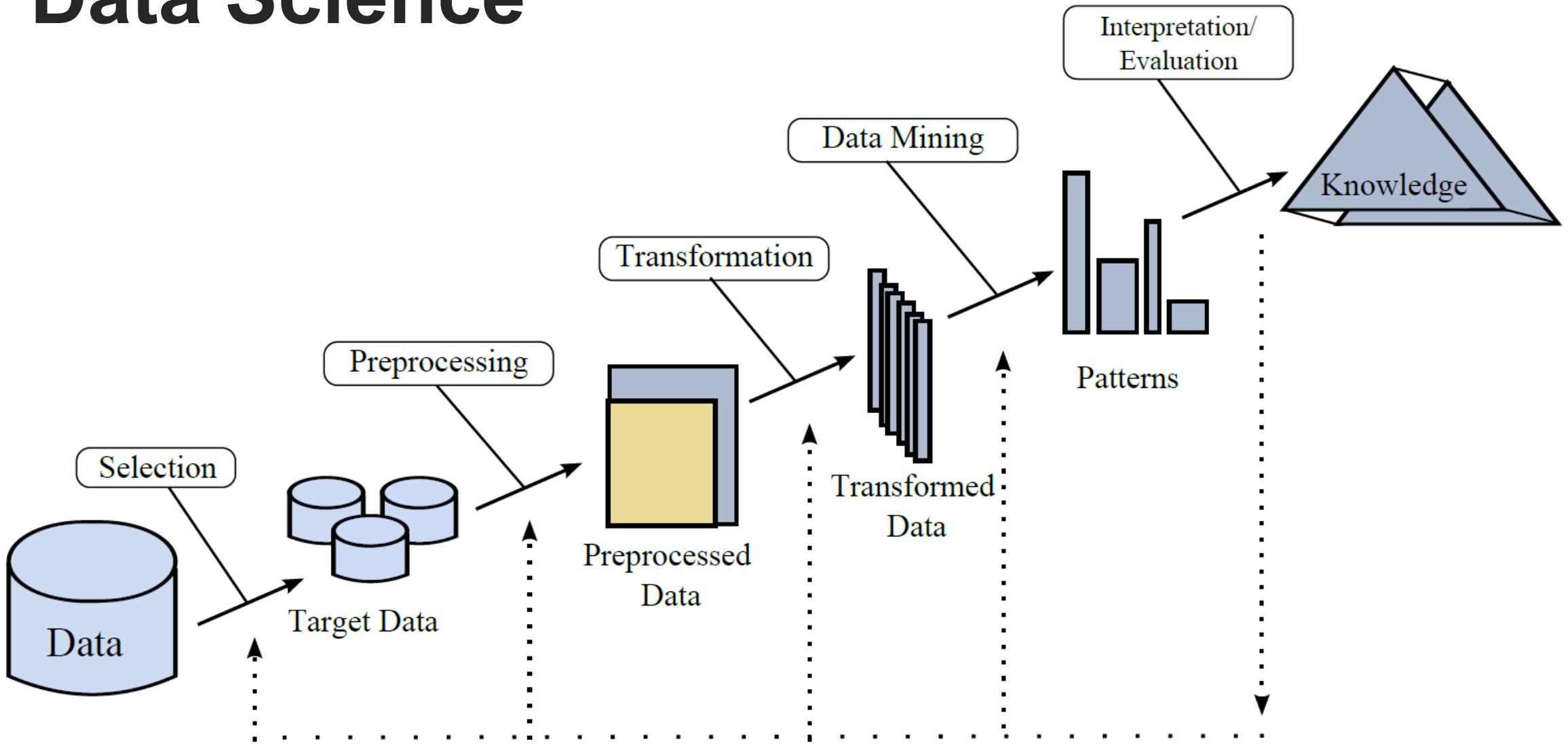
# Deep Learning

Source: <https://becominghuman.ai/building-an-image-classifier-using-deep-learning-in-python-totally-from-a-beginners-perspective-be8dbaf22dd8>





# Data Science



# Optimization



# Optimization

to solve a **problem** that has a number of influencing factors that **need to attain certain value** in order to offer a **solution**

# Applications of AI

1. Engineering
2. Pharmacy & Drugs
3. Environment (Physiology & Architecture)
4. Civil Engineering
5. Physics
6. Biology
7. Hydrology
8. Climate Science

# **Electronics Engineering**

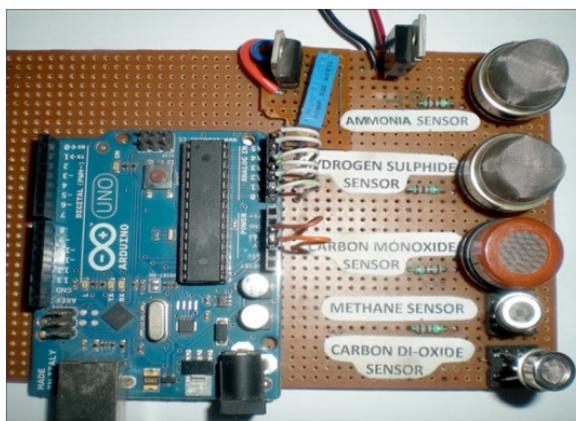
**Protection of health and life of sewer pipeline workers**

# Pattern Recognition

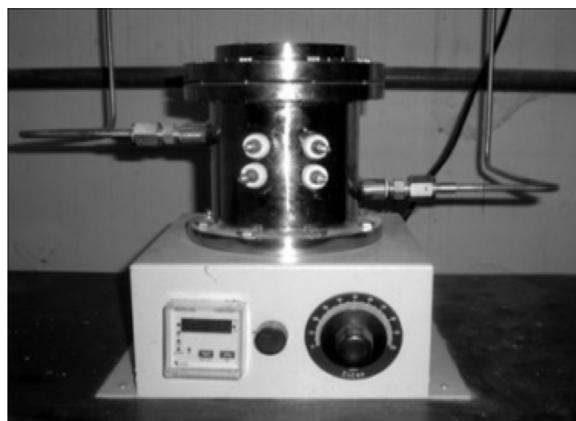
**Intelligent recognizer for the component analysis of toxic mixture of (sewer) gases**



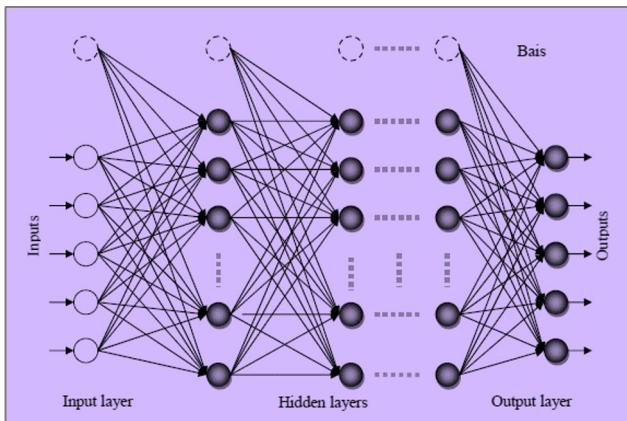
Gas mixture collection



Sensor array formation



Data collection and simulation

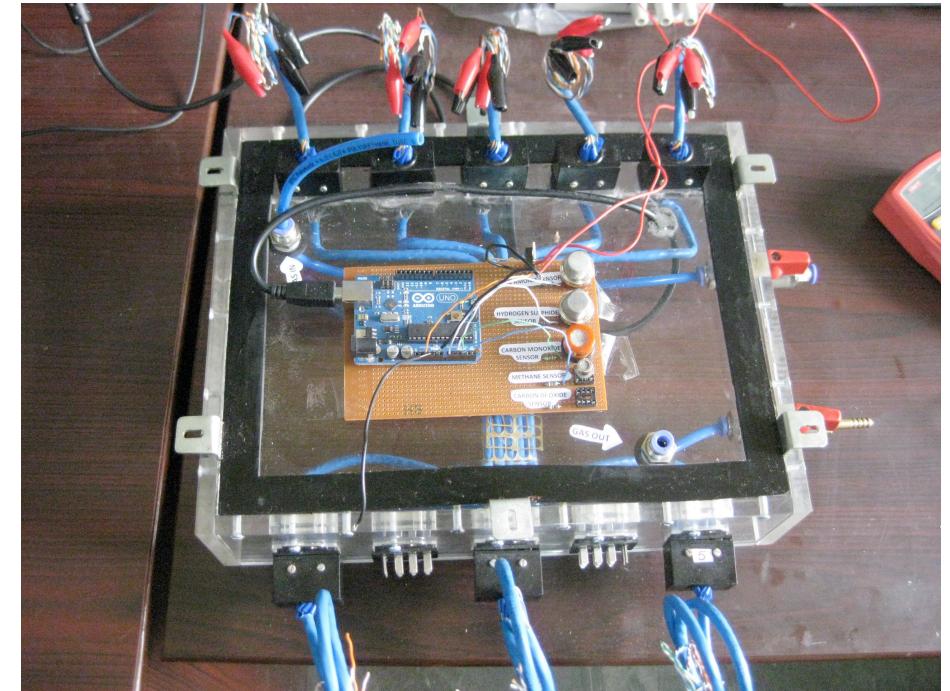


Pattern Recognition

# Prototype of Intelligence Sensor



This was the objective  
☺



We managed to get this one  
nonetheless! (2011-2013)

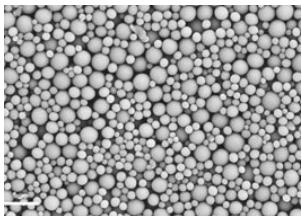
# **Pharmaceutical**

## Drug manufacturing process variables and drug property analysis

# Pharmaceutical (Drugs Production)



# Pharmaceutical



## Powder Properties

(Flowability,  
compactibility) +  
(Roller gap and roller  
speed)

## Particle Properties

(Material type,  
density, size,  
shape and etc.)

## Ribbon Properties

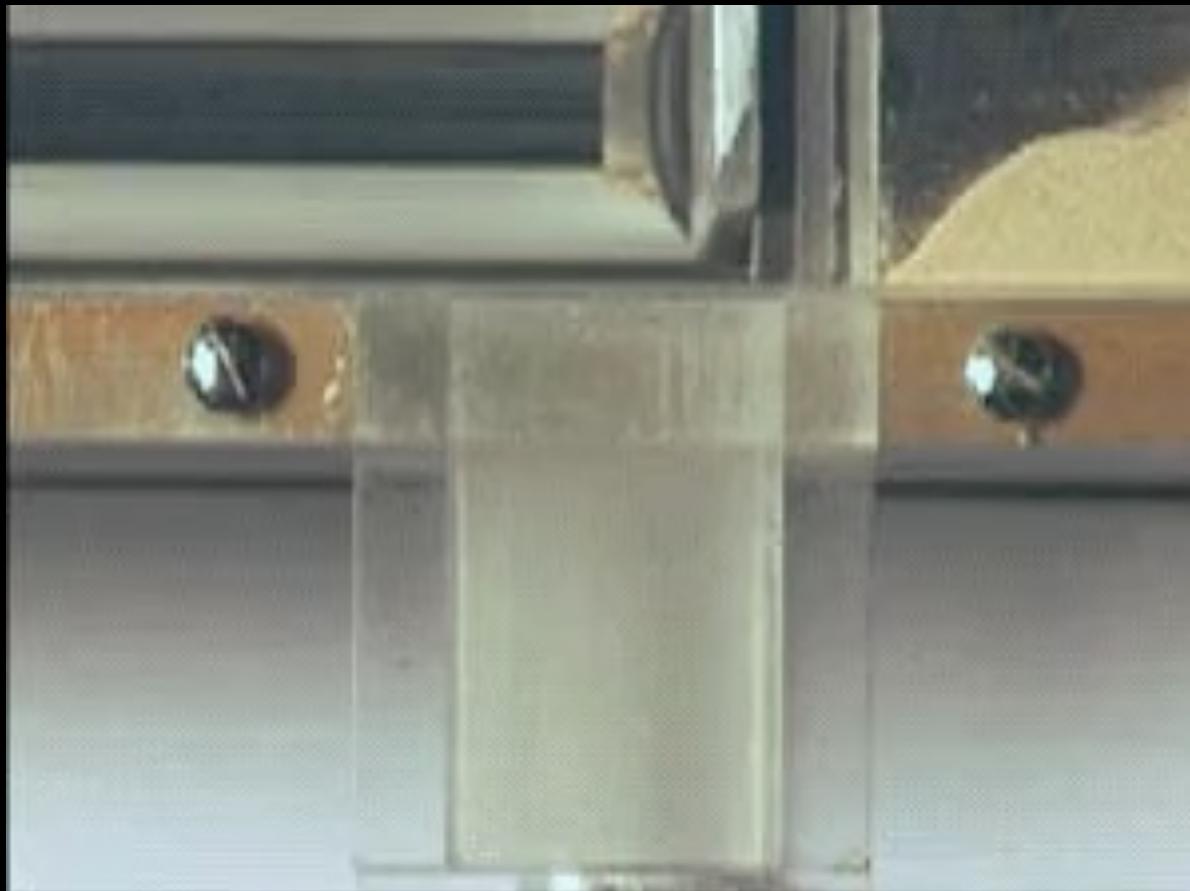
(Density, Hardness,  
Porosity) + (Milling  
speed etc.)

## Granule Size Distribution + (die filling process)

## Tablet Properties (Compressibility)

# Variable Identification of Pharmaceutical Industrial Processes

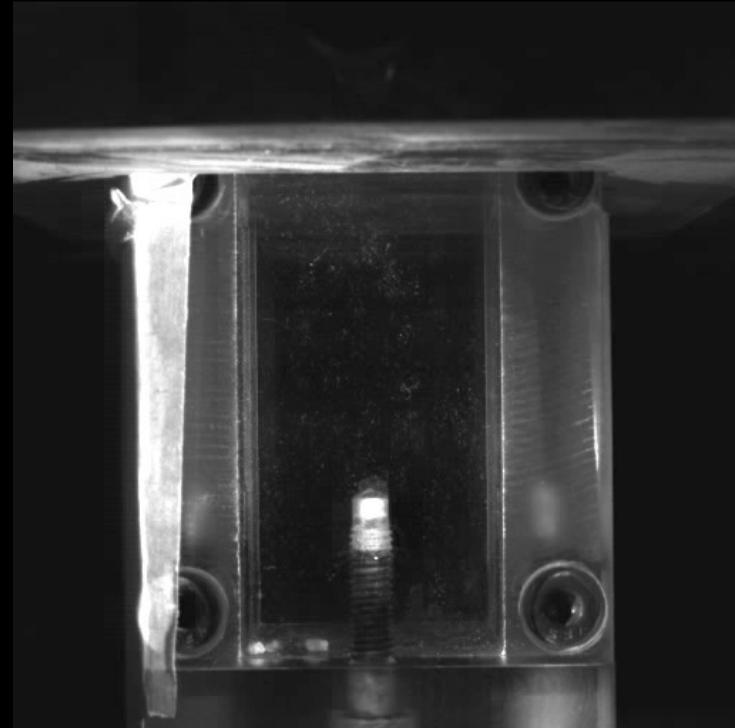
Prediction of the mass of deposited drug powder



**Photron**

1000 fps  
End  
Date : 2015/1/14

FASTCAM SA4 mode...  
1/1000 sec 512 x 512  
frame : -1150 -1150 ms  
Time : 19:41



# Drug Dissolution

Ojha VK et al. (2015) International Journal of Nanomedicine



# Three Hundred Descriptors of Drug Properties

PLGA: poly(lactic-co-glycolic acid)

SI No	Group name	No of features	Importance
1	Protein descriptors	85	Describes the type of molecules and proteins used
2	Formulation characteristics	17	Describe the molecular properties such as molecular weight, particle size, etc
3	Plasticizer	98	Describe the properties such as fluidity of the material used
4	Emulsifier	99	Describe the properties of stabilizing/increase the pharmaceutical product life
5	Time in days	1	Time taken to dissolve
6	% of molecules dissolved	1	Output

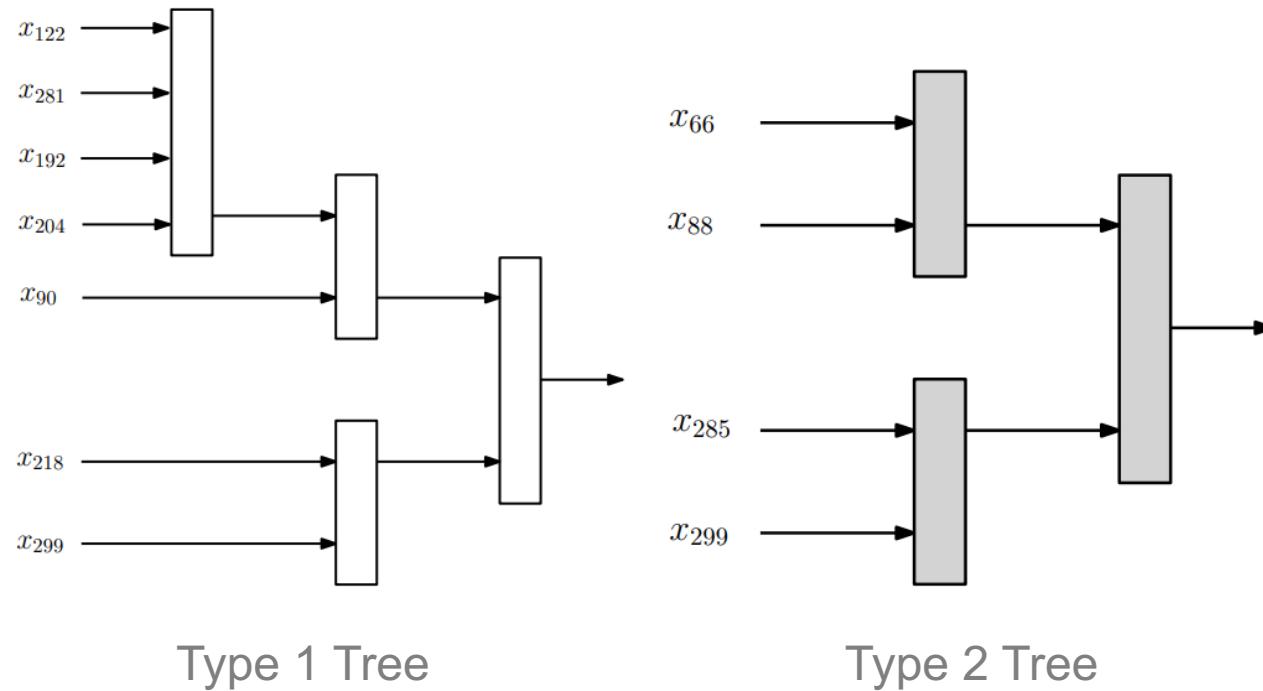
**Abbreviations:** PLGA, poly(lactic-co-glycolic acid); SI, serial; No, number.

# Balancing Prediction and Feature Selection

Algorithm	RMSE $E_t$	No. of features
MLP	14.3	17
<b>Neural Tree</b>	13.2	15
REP Tree	13.3	15
GPR	14.9	15
MLP	15.2	15
MLP	15.4	11
<b>Type 1 Tree</b>	18.6	7
<b>Type 2 Tree</b>	15.2	4

# A Tree Model for Future Use

Can we also explain how the prediction was made?

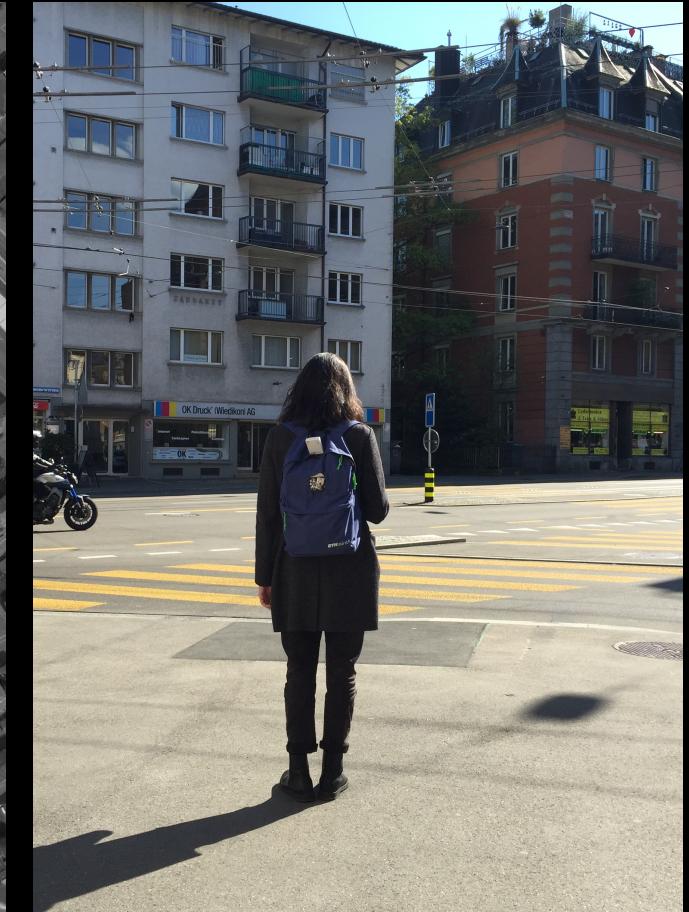


If protein is A and plasticizer is B, Then % molecule dissolution is X

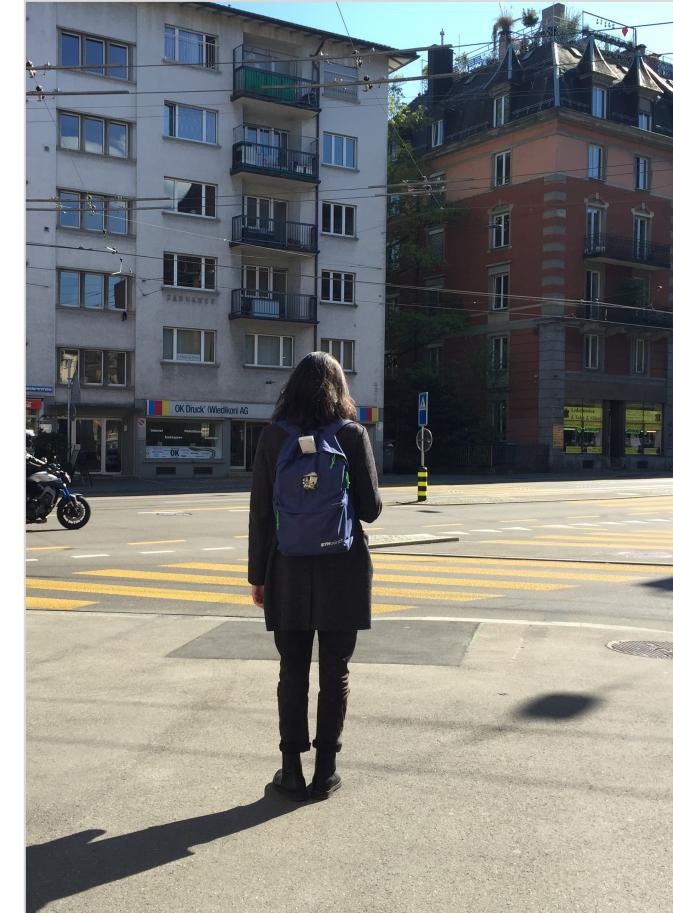
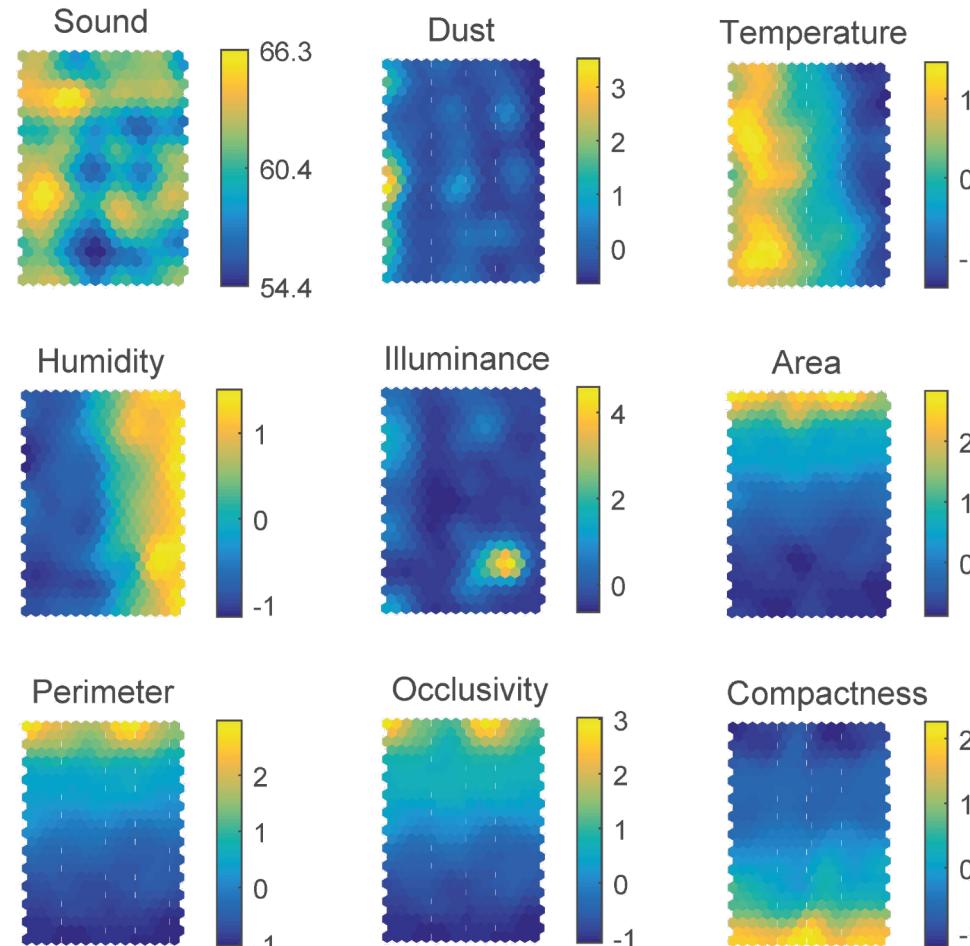
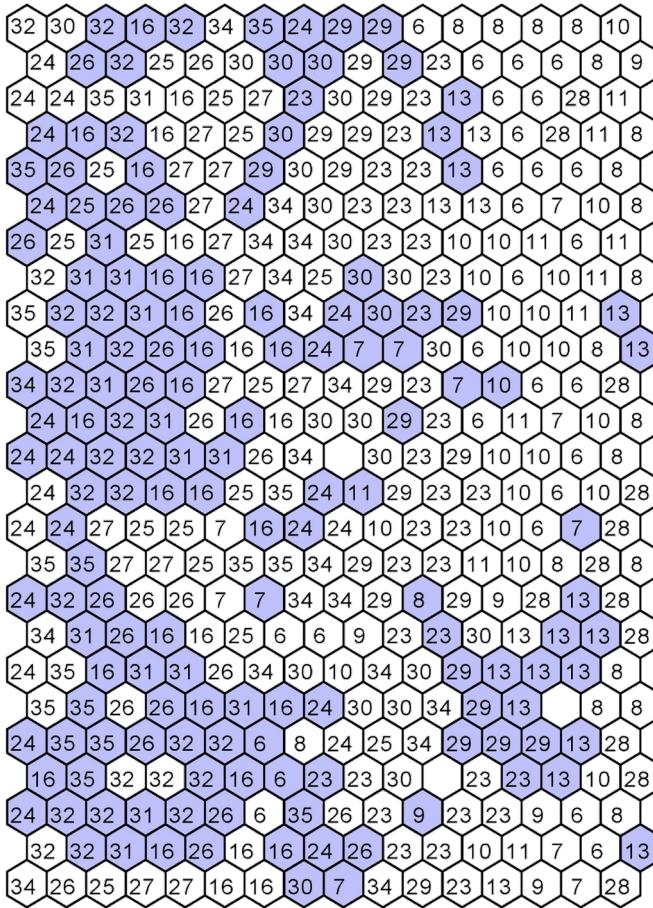
# **Build Environment**

Understanding impact of environment and urban  
dynamics on humans

# Perception of the Environment



# Perceptual Experience



# Civil Engineering

## Structure buckling analysis

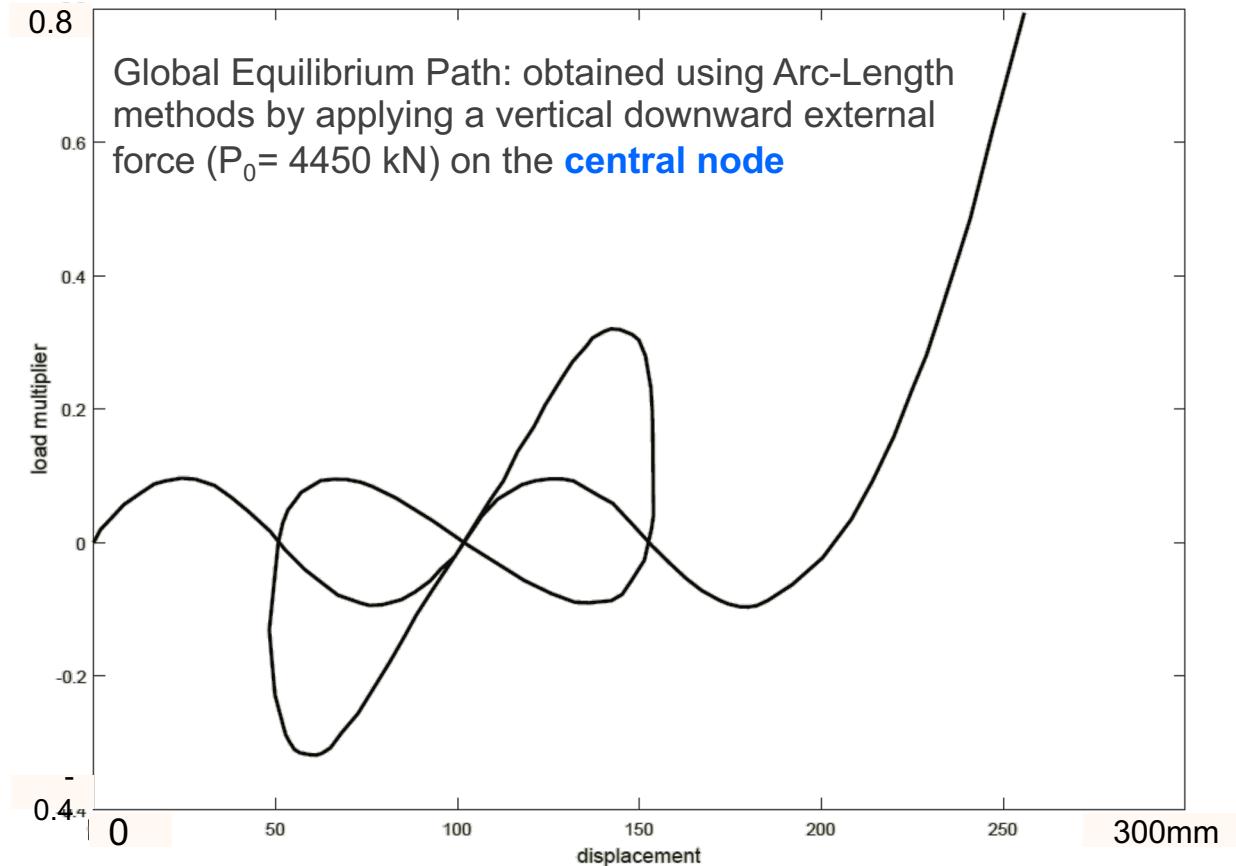
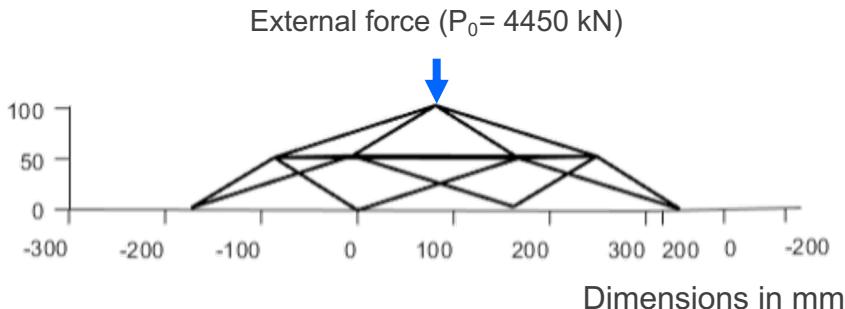
# Civil Engineering Problem



# Civil Engineering Problem

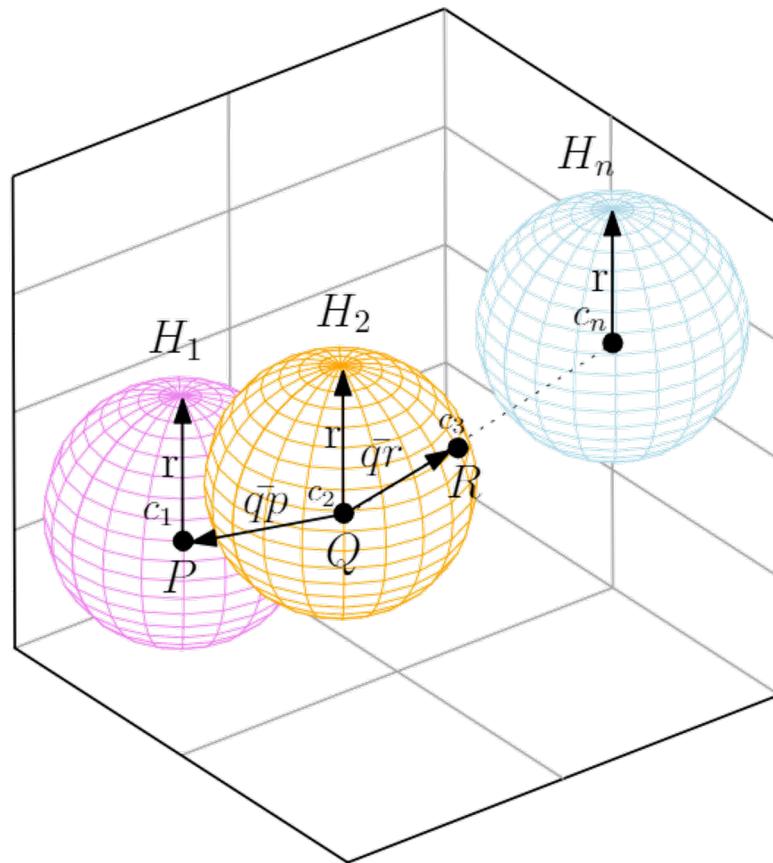


A tiny version of Millennium Dome can be the following structure

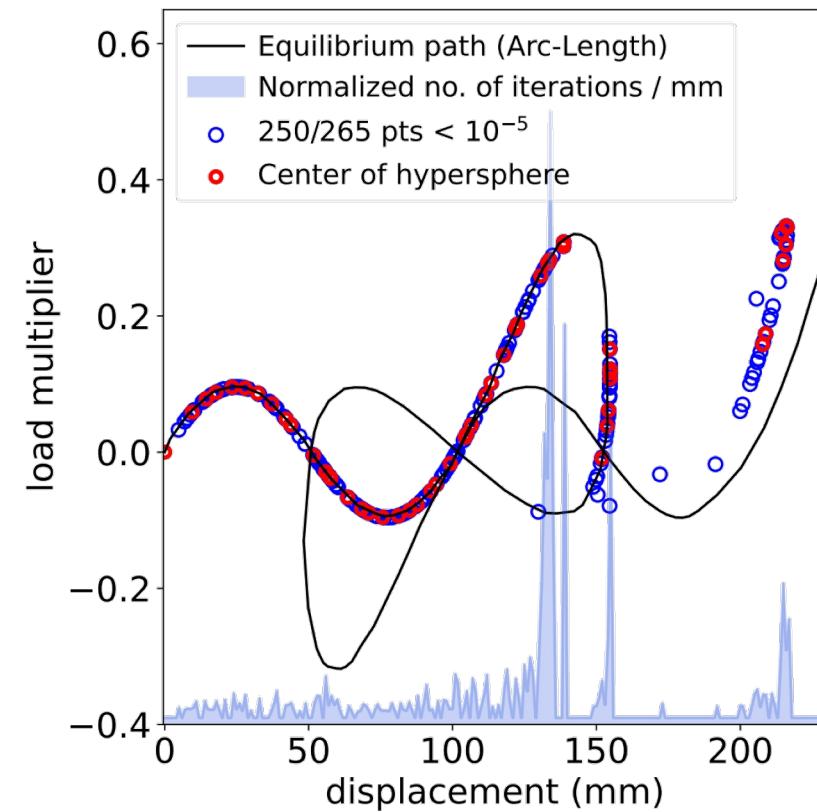


Hrinda, G. (2010, April). Snap-through instability patterns in truss structures. In 51st AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference 18th AIAA/ASME/AHS Adaptive Structures Conference 12th (p. 2611).

# Civil Engineering Problem

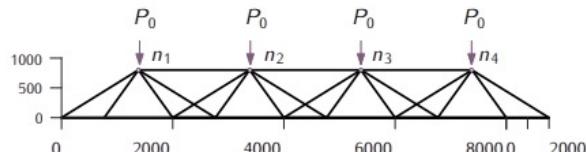


**Fig A.** Adaptive Hypersphere Search Algorithm for Structural Static Analysis

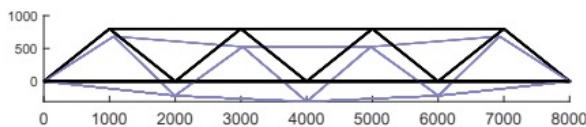


**Fig B.** Equilibrium Path traced using Adaptive Hypersphere Search Algorithm

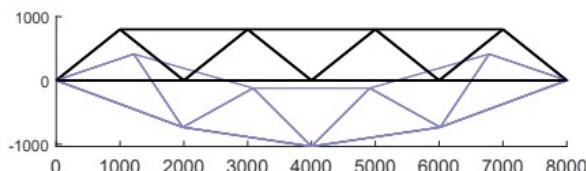
Side view (2D view)



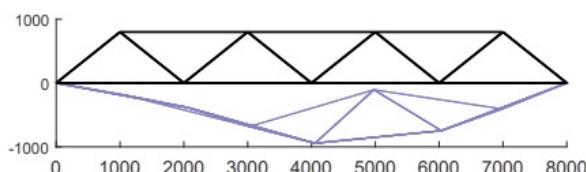
Undeformed shape



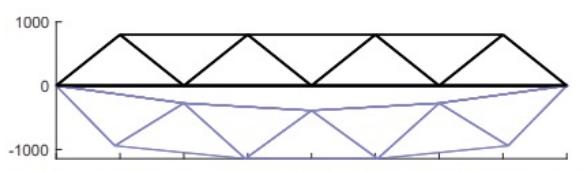
Deformed shape A



Deformed shape B

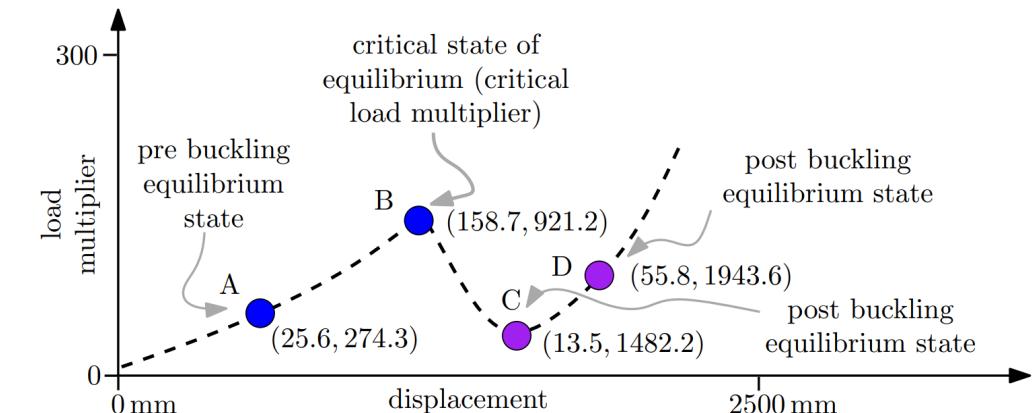
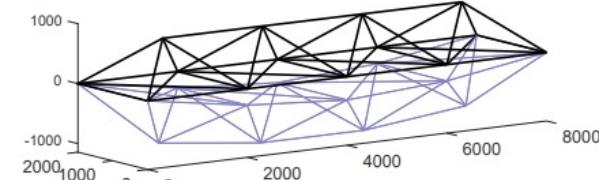
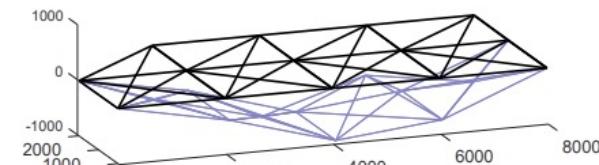
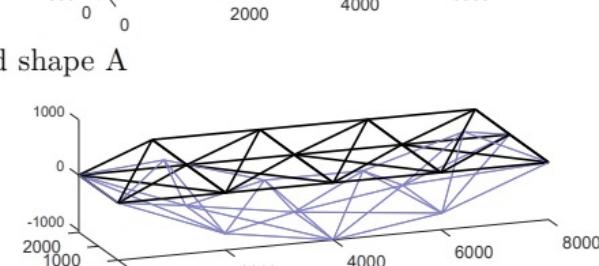
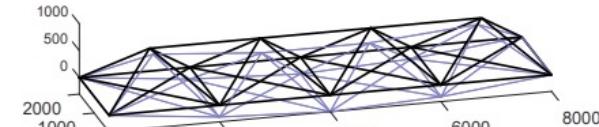
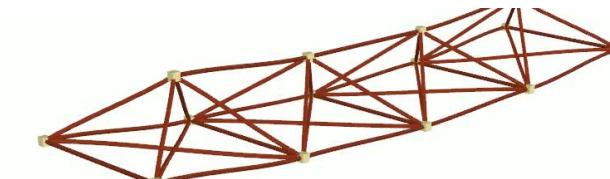
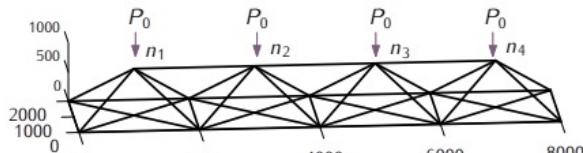


Deformed shape C



Deformed shape D

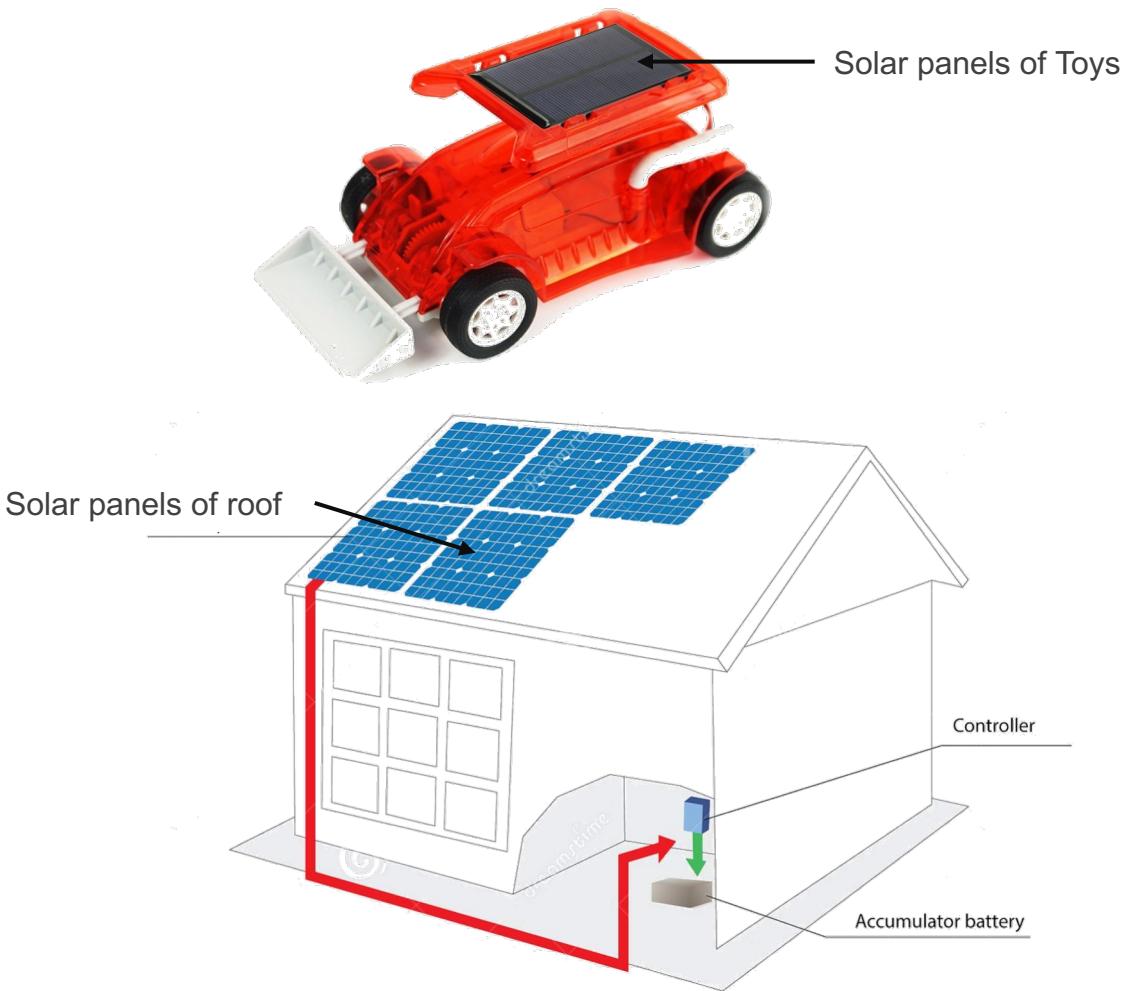
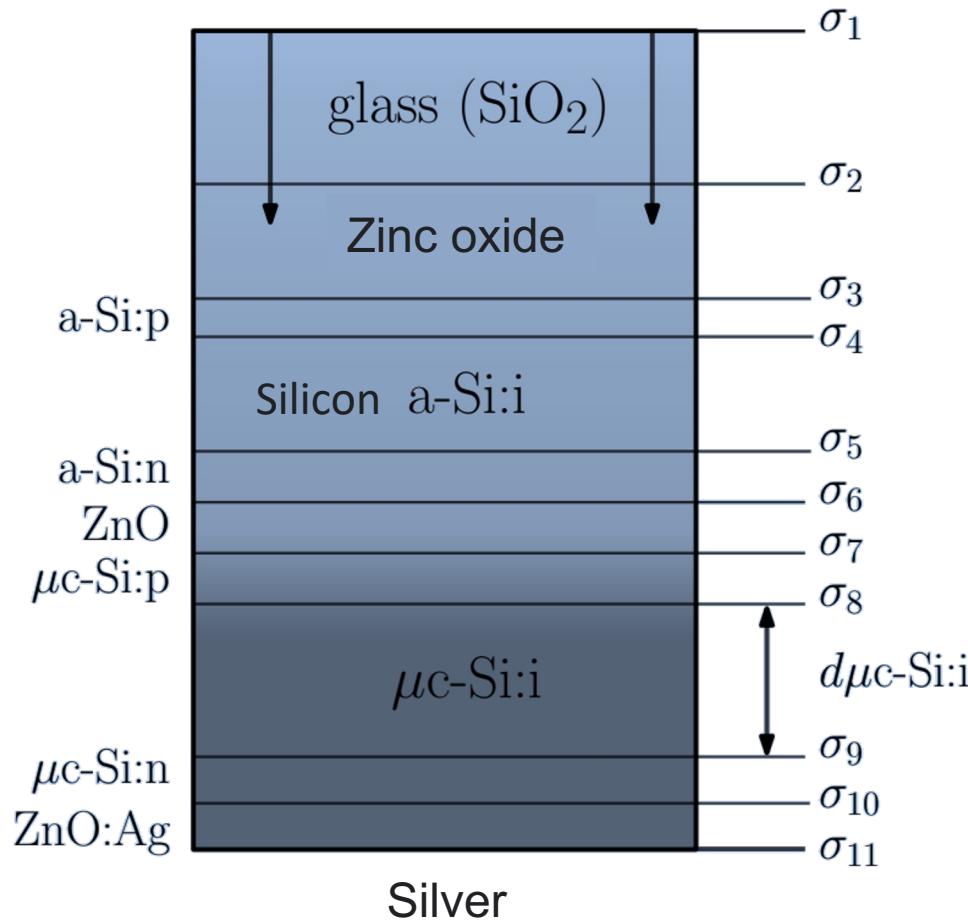
Top view (3D view)



# **Physics**

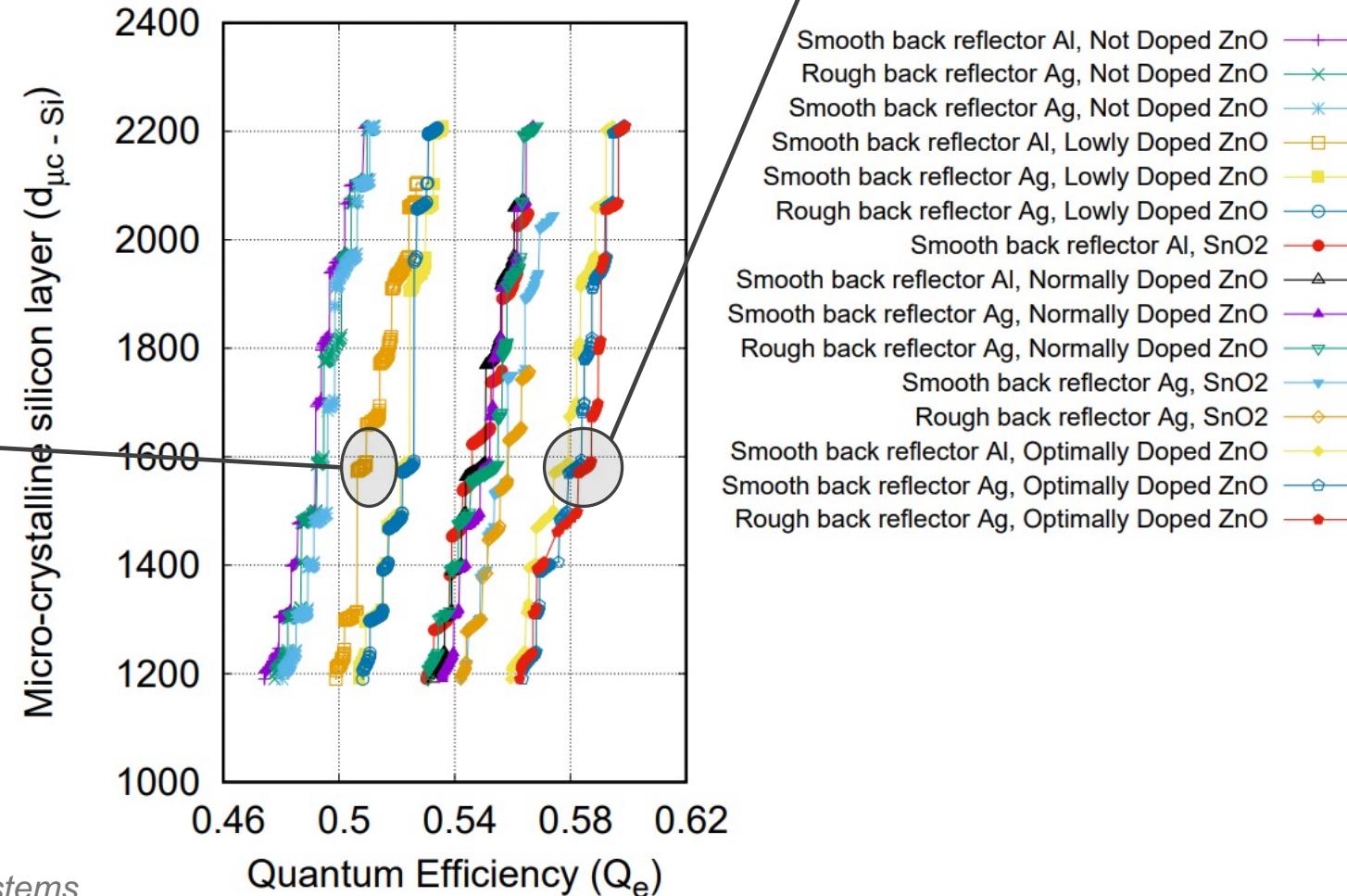
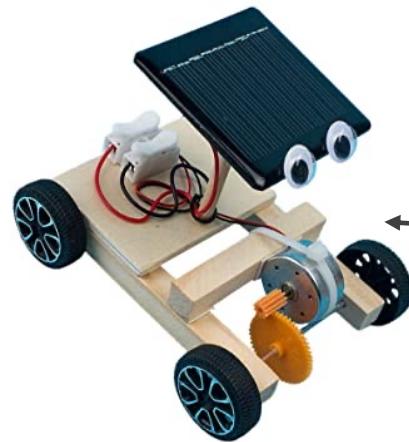
## Solar cell design and characterization

# Solar Cell – Energy Optimization



# Solar Cell

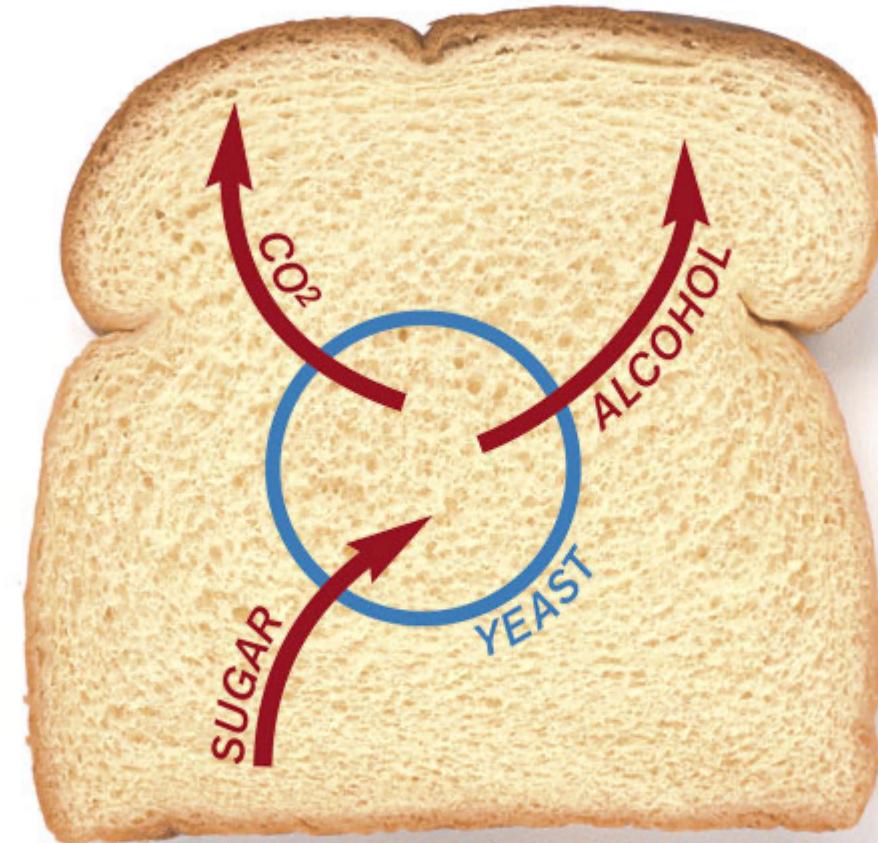
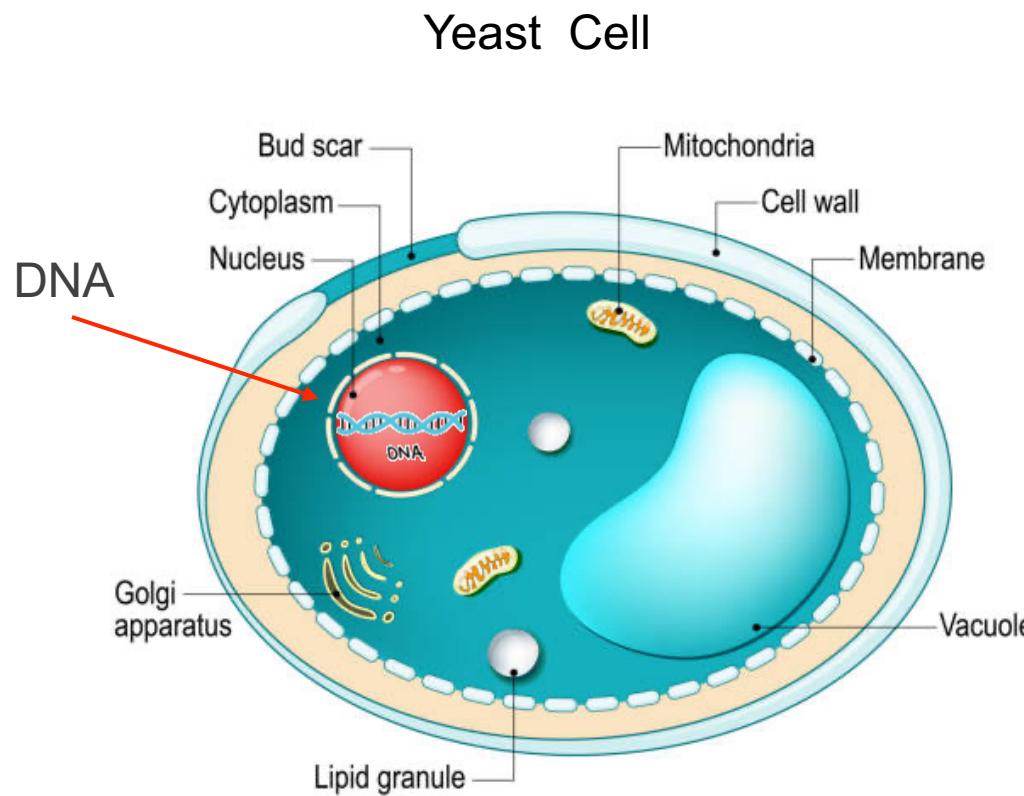
## Cost and Efficiency Trade-offs for its Usage

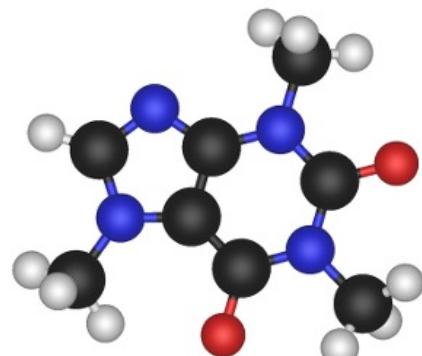


# Biology

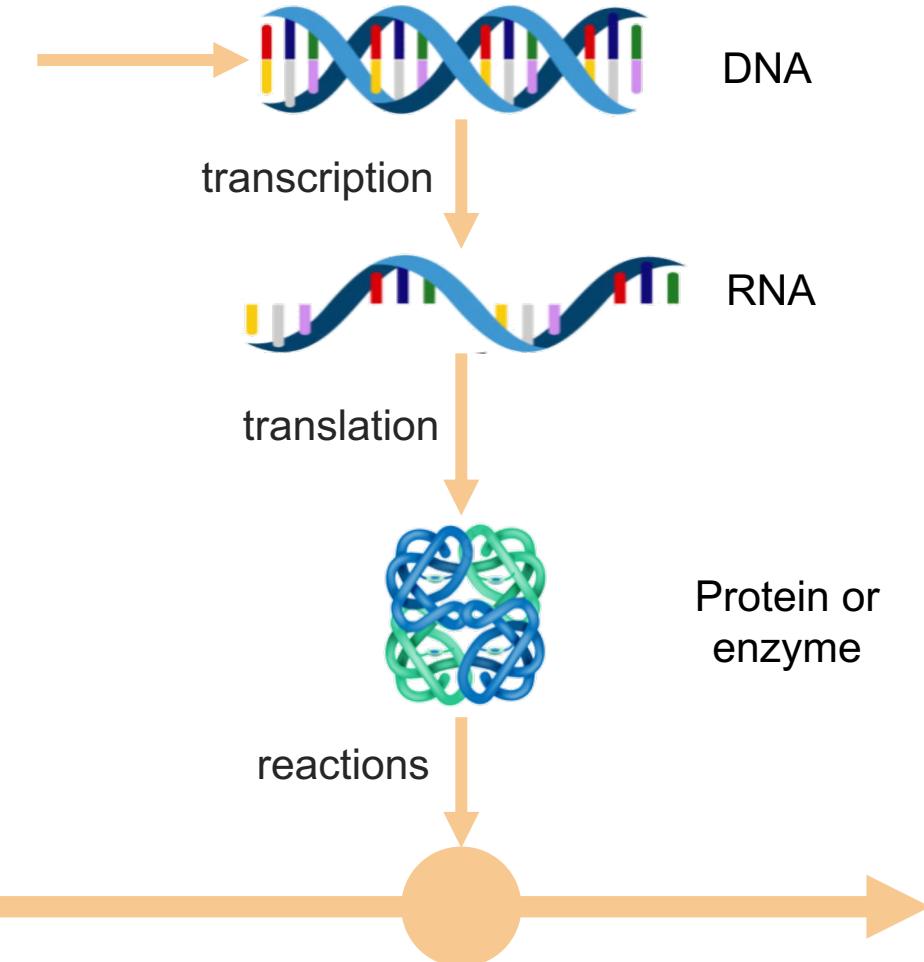
Metabolic engineering (searching for best strains)

# Role of Yeasts in Food Production

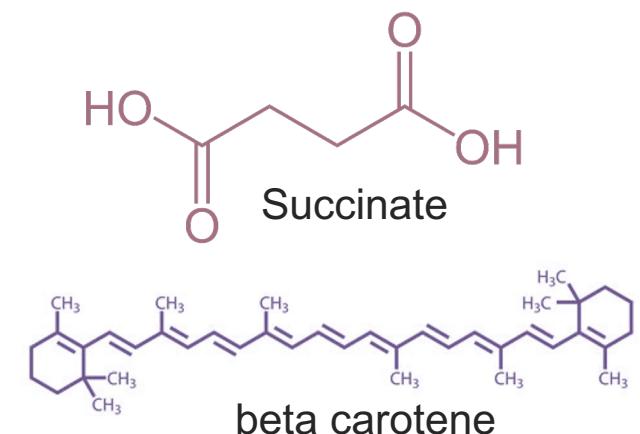




## Metabolic Engineering

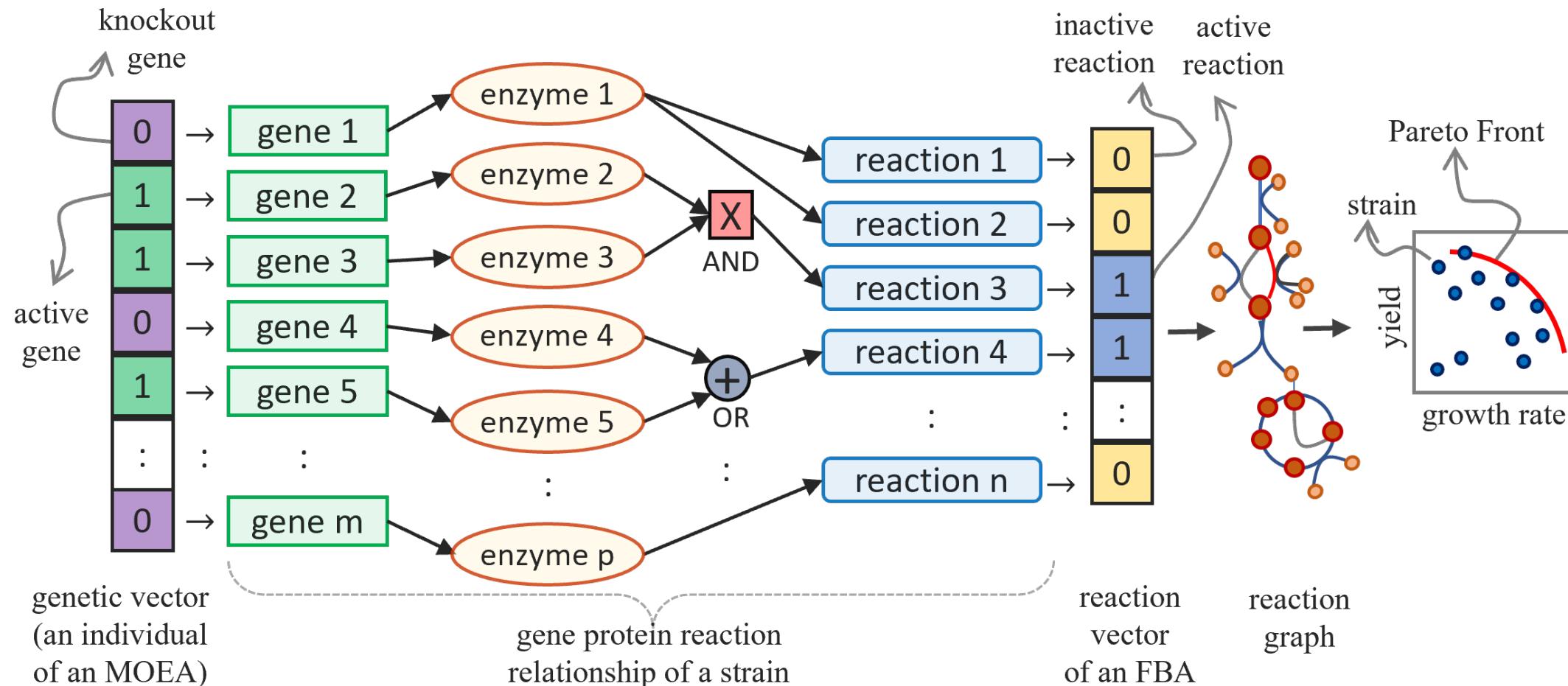


Molecular Structure of  
Ordinary Chemicals

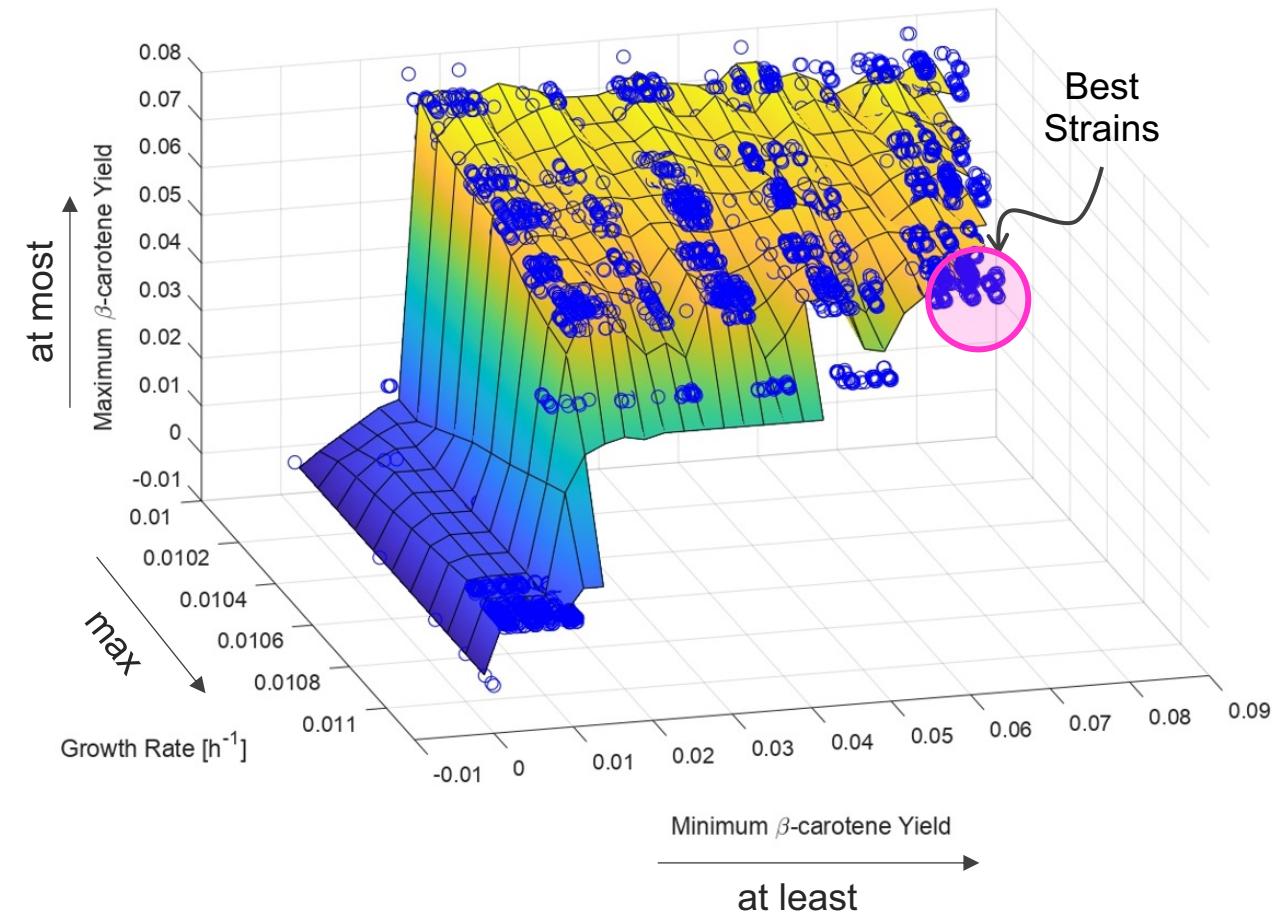
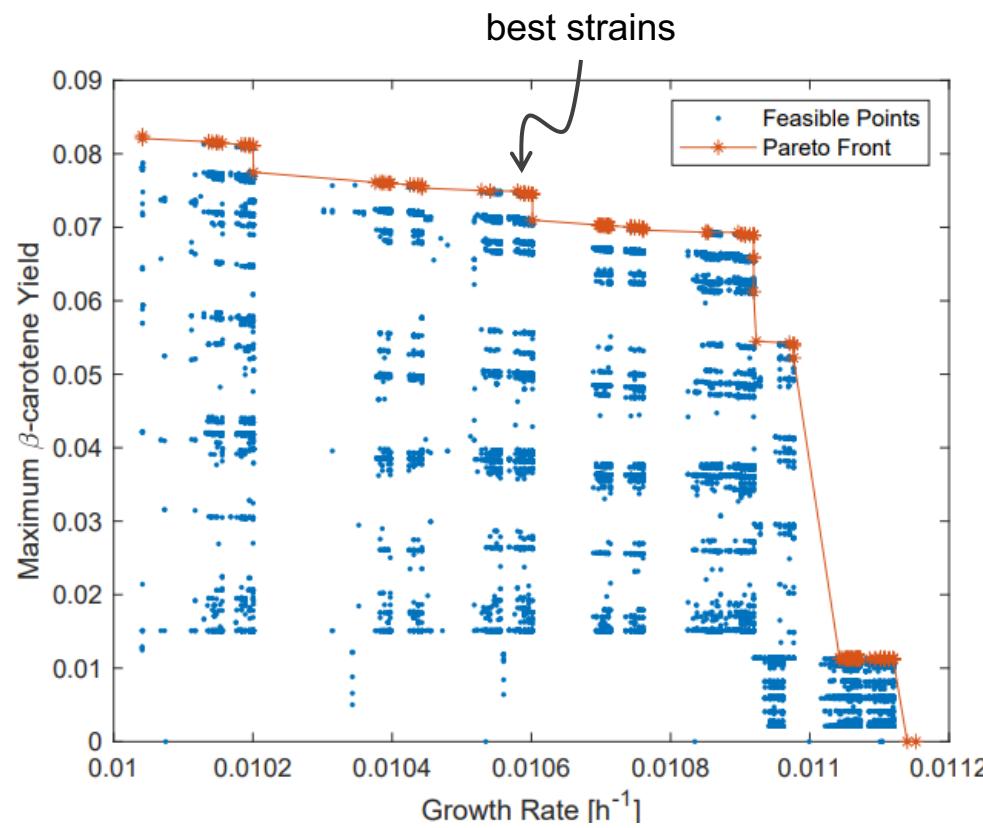


Molecular Structure of Target  
Chemicals

# Metabolic Engineering for Chemical Production



# Optimal Strains of Yeast

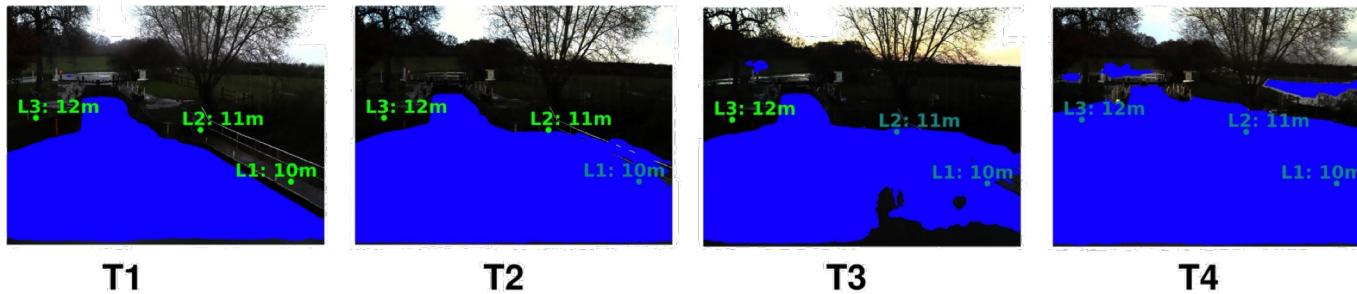


# Hydrology

Prediction of flood events

# Hydrology: Flood Event Prediction

A collaboration with Meteorology (Prof. Sarah Dance and Remy Vandaele)



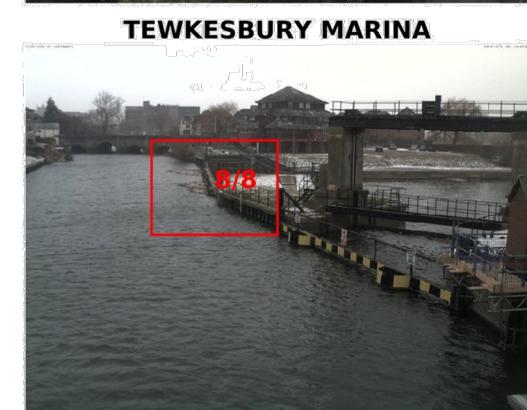
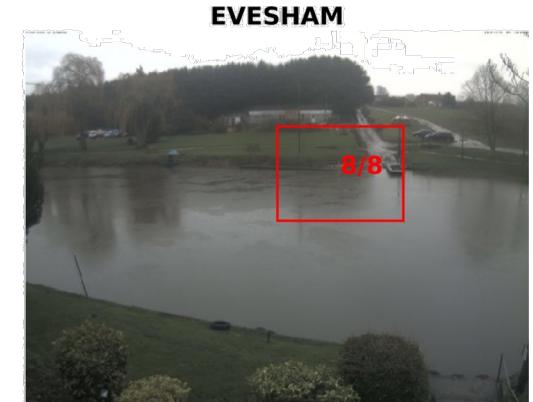
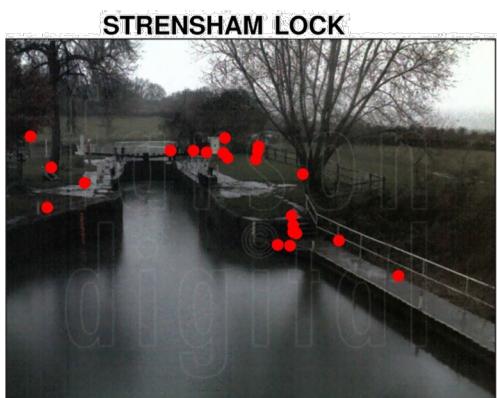
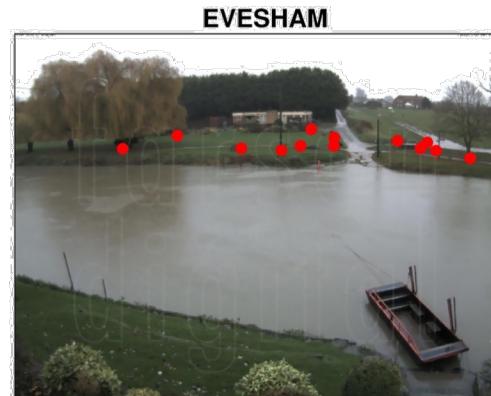
**Fig.** Time-series sequence of images of river. Blue pixels are water segmentation by using deep learning models



Credit: Farson Digital Watercams  
[https://www.farsondigitalwatercams.com/locations/keswick\\_greta](https://www.farsondigitalwatercams.com/locations/keswick_greta)

# Hydrology: Flood Event Prediction

A collaboration with Meteorology (Prof. Sarah Dance and Remy Vandaele)



**Fig A.** Customized dataset:  
Landmark annotation of waterline

Vandaele, Dance, and Ojha, (2021) *Hydrology and Earth System Sciences*

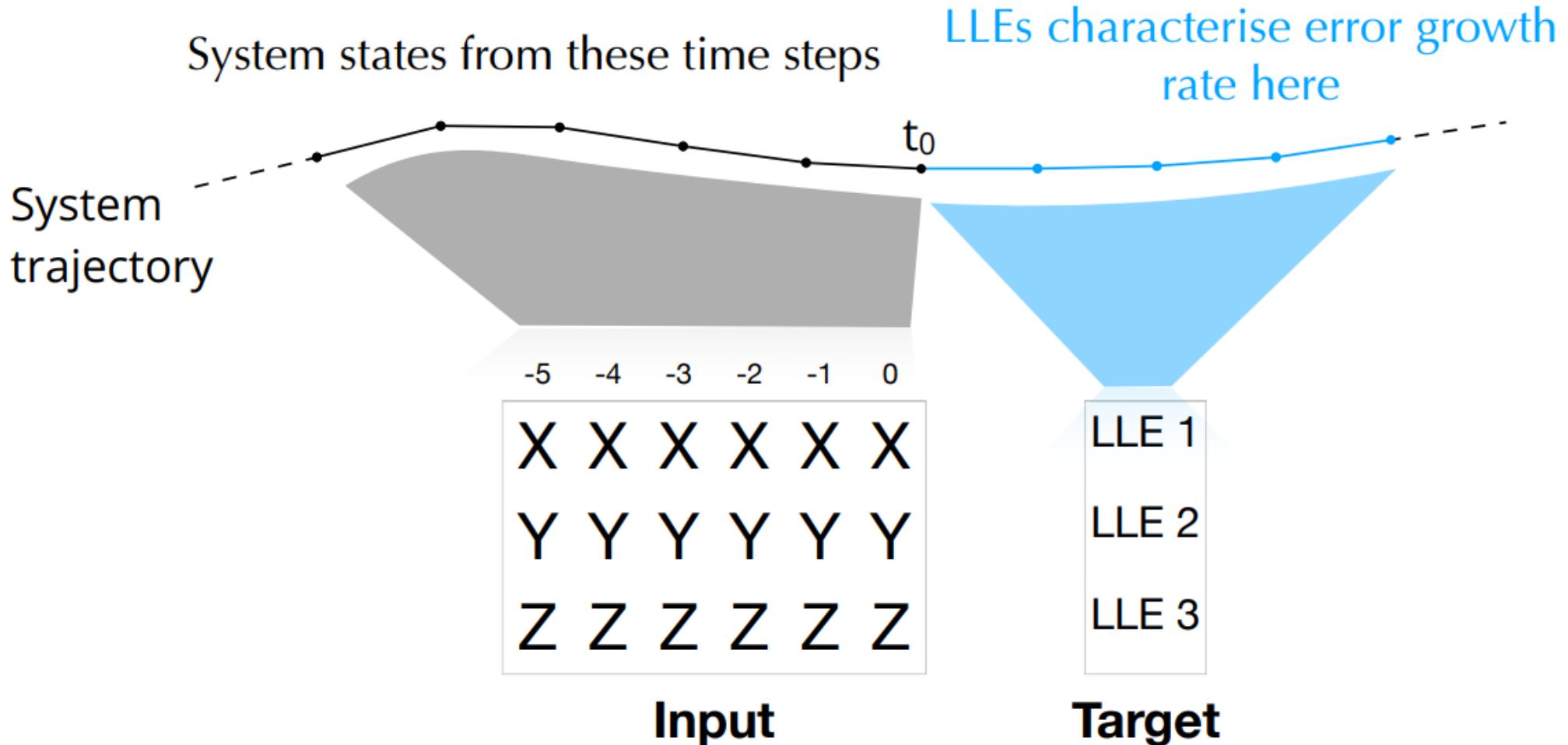
<https://doi.org/10.5194/hess-25-4435-2021>

**Fig B.** Best window identification for prediction accuracy.  
We achieve 94% accuracy in correctly predicting real flood events.

# **Climate Science**

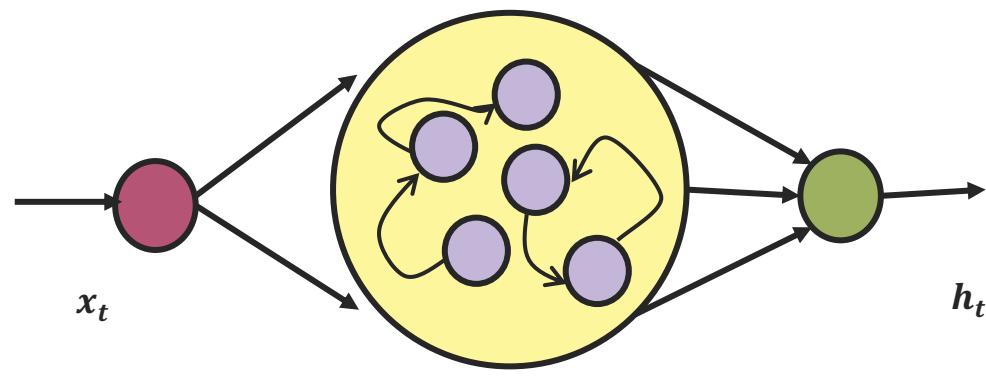
**Non-intrusive modelling of dynamical systems**

# Predicting Instabilities in Chaotic Systems

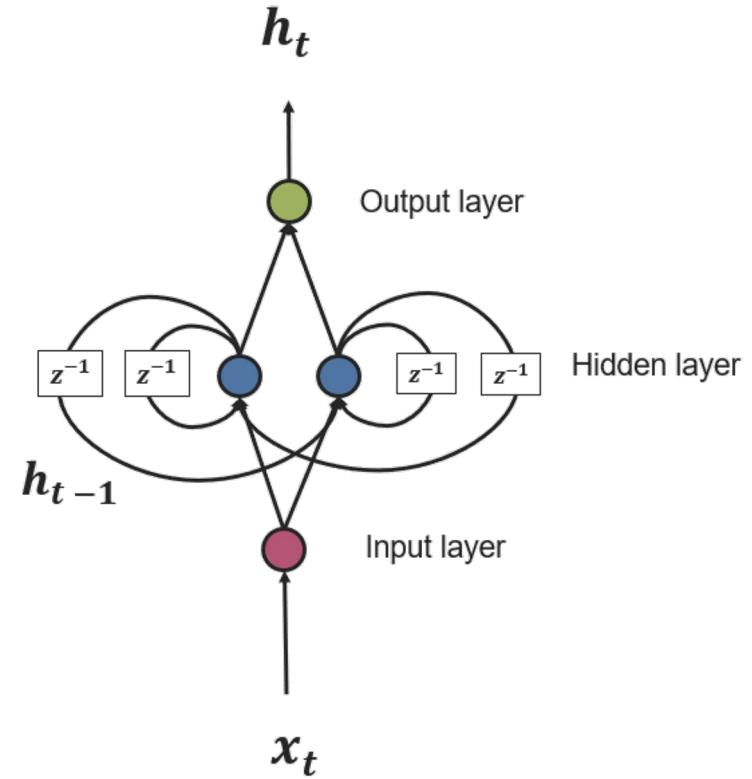


# Machine Learning Algorithms to Use

Supervised **recurrent neural networks** for the reconstruction short term dynamics



Eco State  
Network



Long Sort Term  
Memory

# What LOSS function can we use?

We can consider two types of losses:

- **Purely Data Driven loss (Neural Nets):**

$$\bullet \text{loss} = \frac{1}{N} \sum (x_{t+1} - f(x_t))^2$$

- **Physics Informed loss (Physics Informed Neural Nets)**

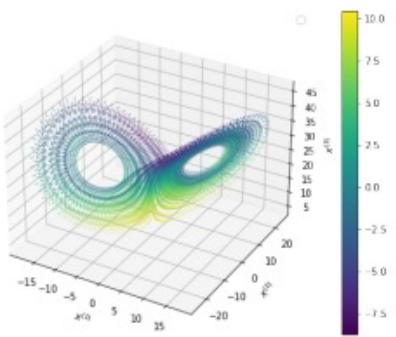
$$\bullet \text{loss} = \frac{1}{N} \sum (x_{t+1} - f(x_t))^2 + \text{physics (e.g., } |RK_4(x_t) - RK_4(f(x_t))|)$$

# Data Driven Neural Nets

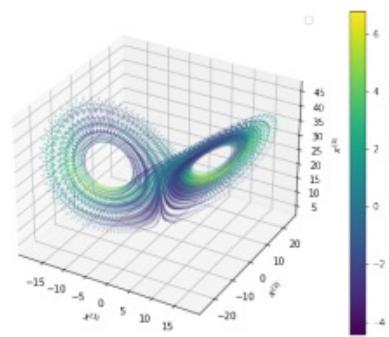
(prediction of short term dynamics )

Rössler 76 Lorenz 63

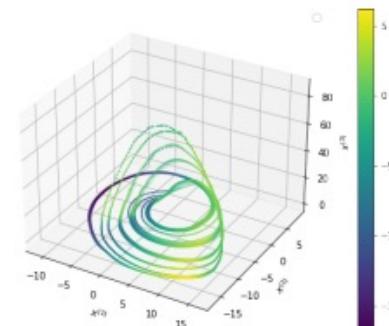
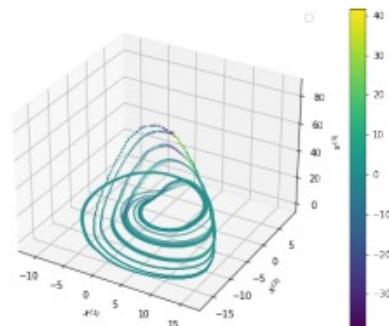
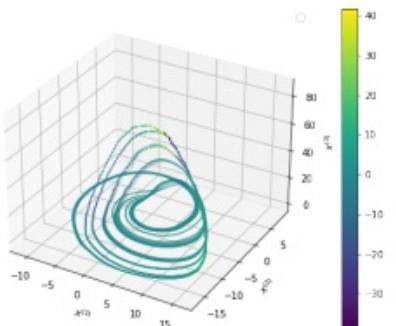
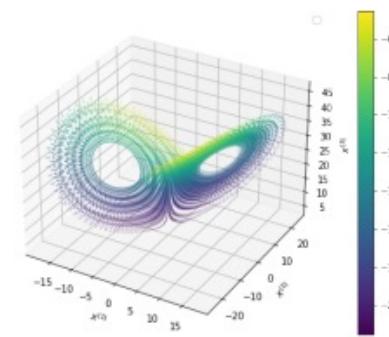
*LLE1*



*LLE2*



*LLE3*

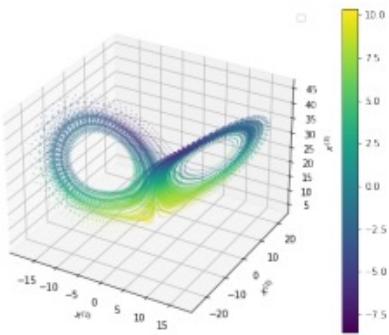


# Physics Informed Neural Nets

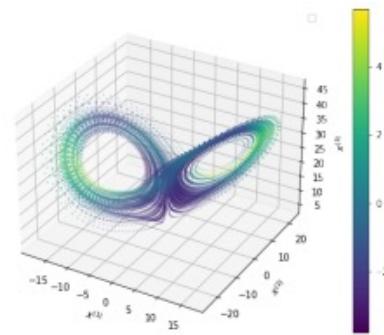
(prediction of short term dynamics)

Rössler 76 Lorenz 63

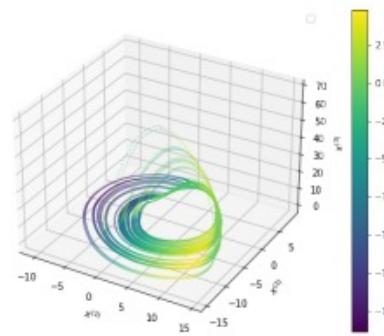
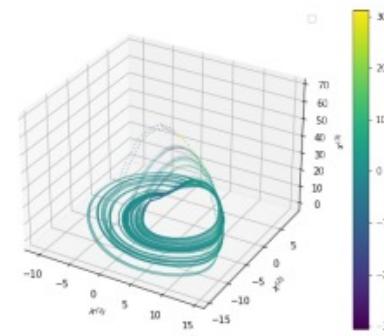
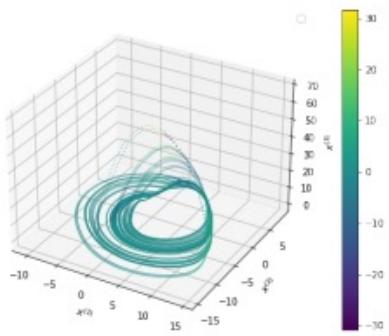
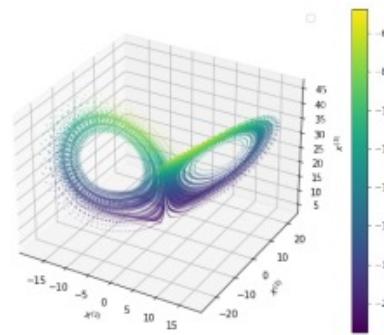
*LLE1*



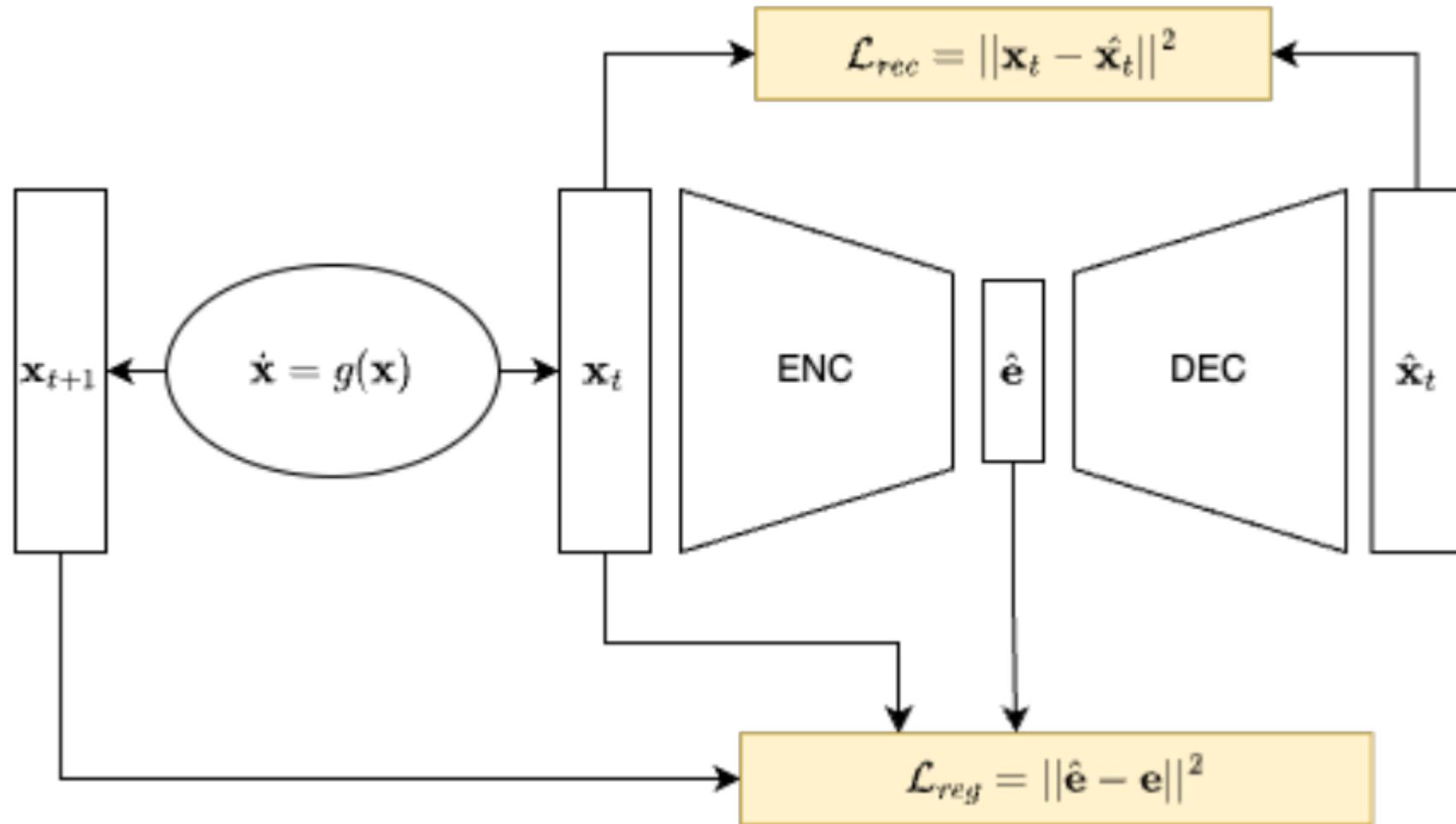
*LLE2*

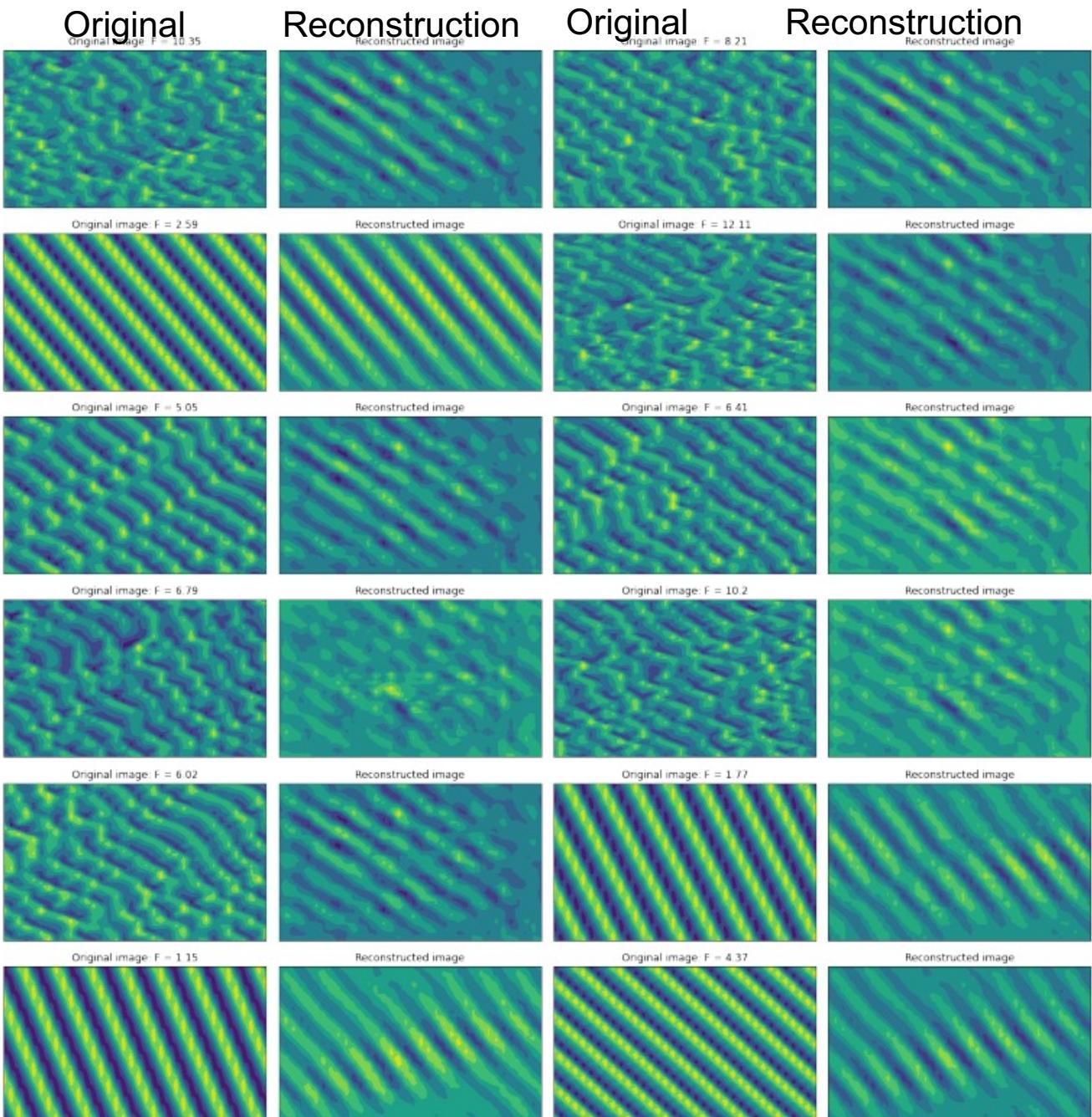


*LLE3*



# Symmetric Convolutional Autoencoder





## Plastic Waste Pollution (Input Video)



155387785

## AI Solution (Output Video)



Jaikumar P et al. (2020) ISDA, <https://centaur.reading.ac.uk/98569/>

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