Using AI to improve our Understanding of Waste-water processing

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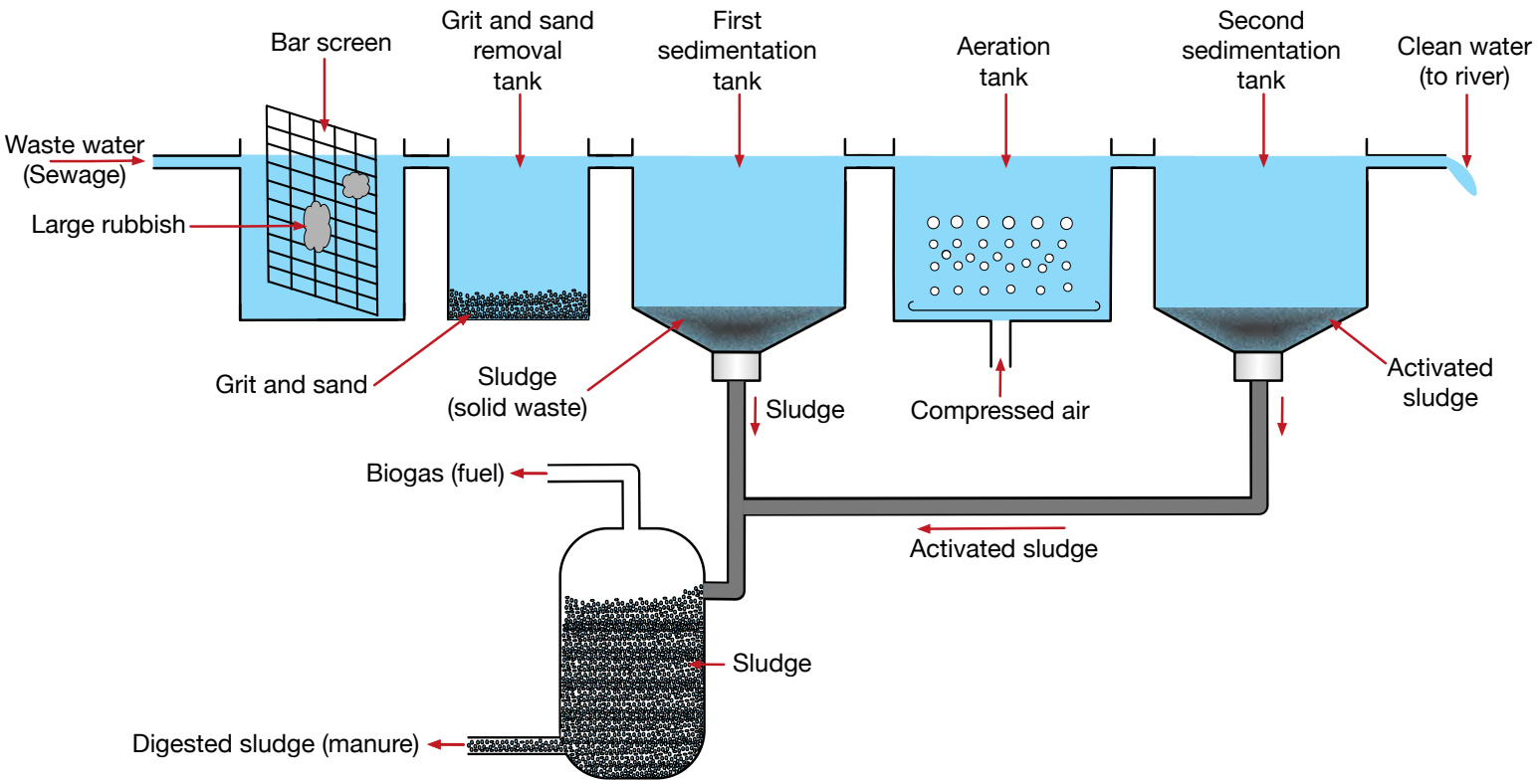
ENBIS Meeting, May 18th, 2021

Outline

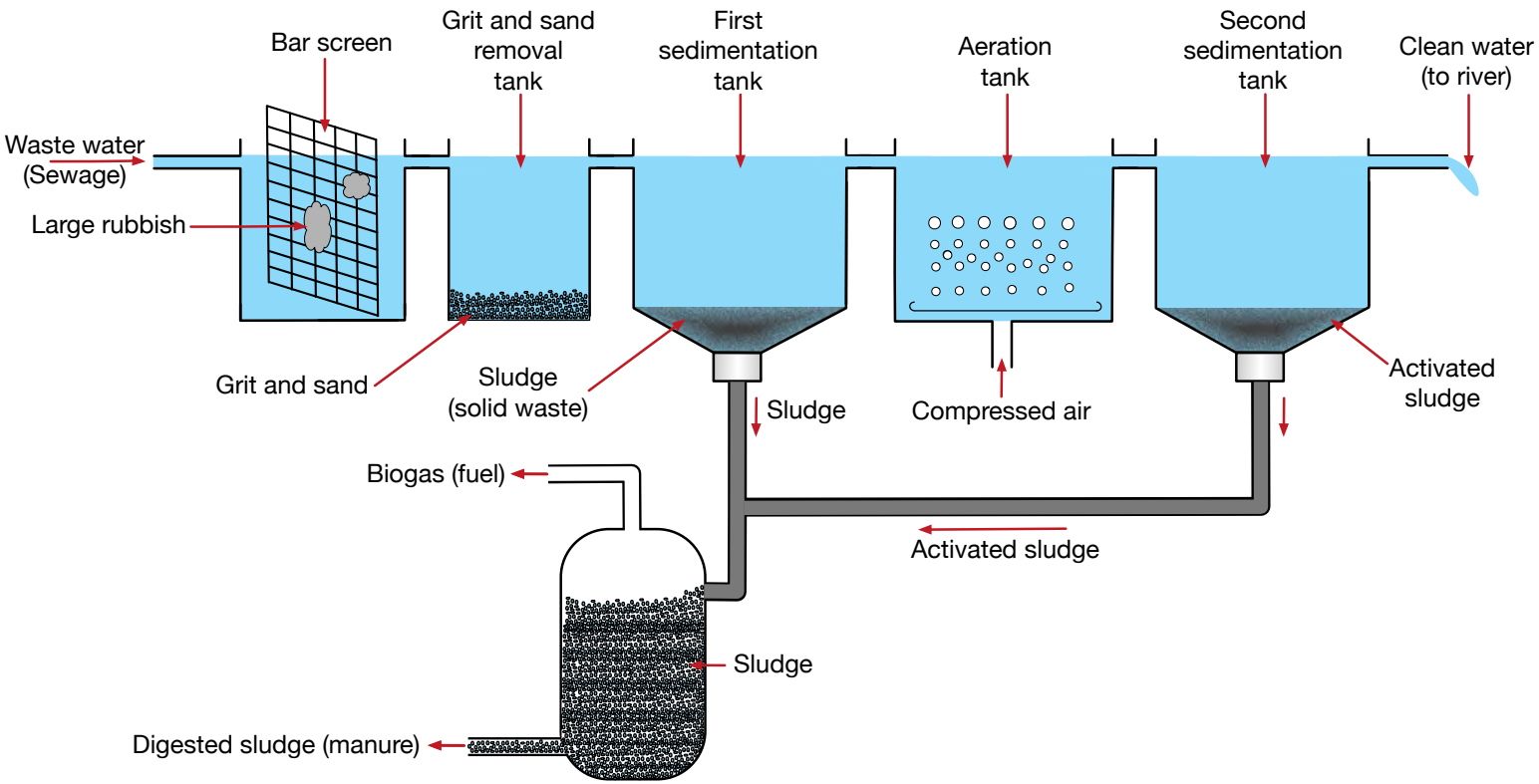
- **Wastewater Treatment Primer**
- Simulating wastewater treatment
- AI Primer
- Using AI for wastewater treatment

Wastewater treatment process



- Process dates back to 1868
- Bacteria in sludge breaks down harmful chemicals
- But new directives require lower levels of contaminates in outflow

Dealing with contaminates



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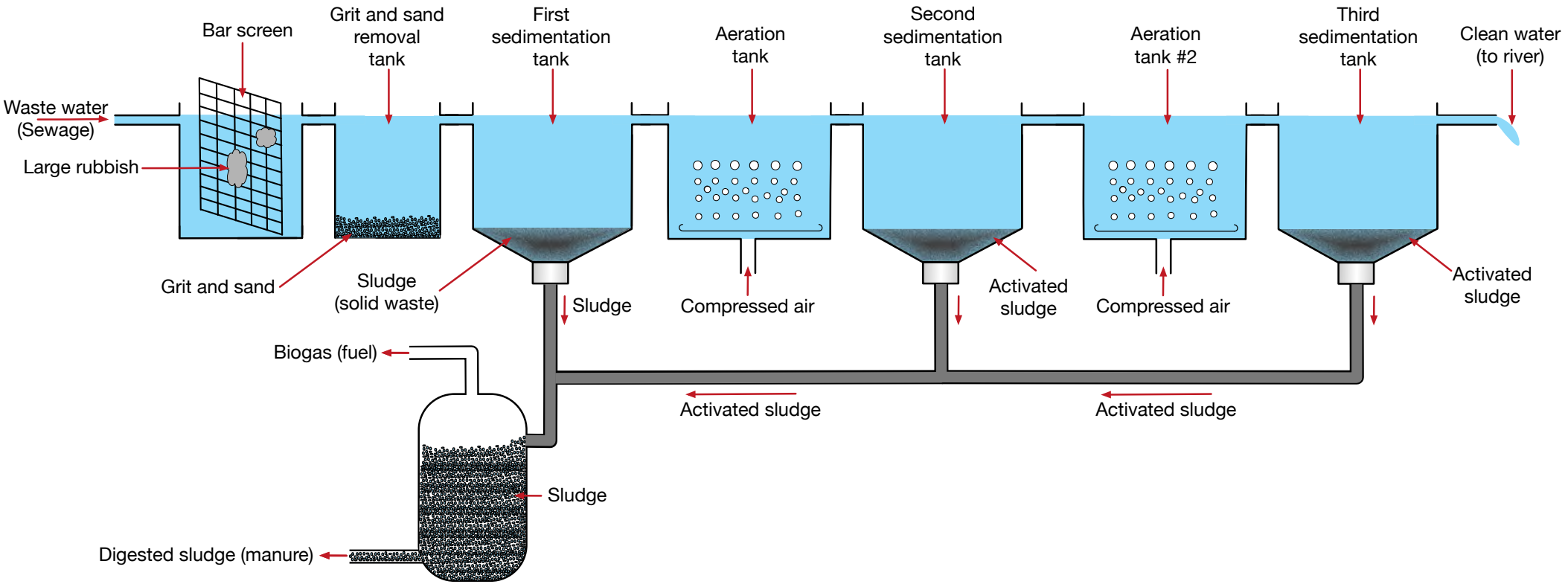

Want to do this ’better’

- No extra energy input
- No need for extra facilities
- How?
  - The bacteria
  - The environment

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- AI Primer
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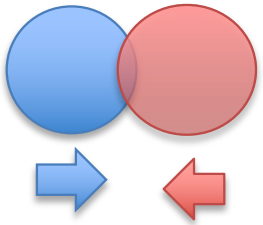
Agent Based Model

- Simulate system – Agent Based Model
- Each bacteria is an agent
  - Acts out the bacteria's biological and mechanical – processes

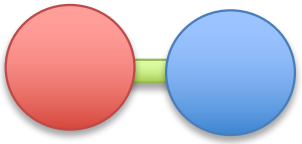
Process Stages

Mechanical Relaxation

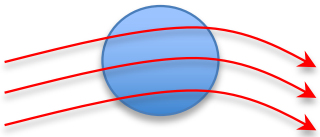
Contact force



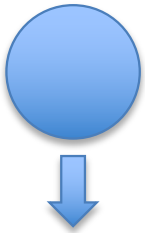
Adhesive force



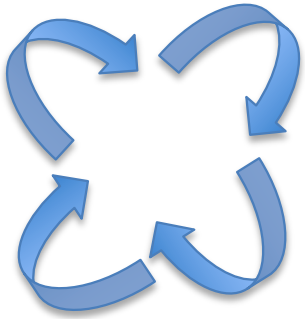
Fluid force



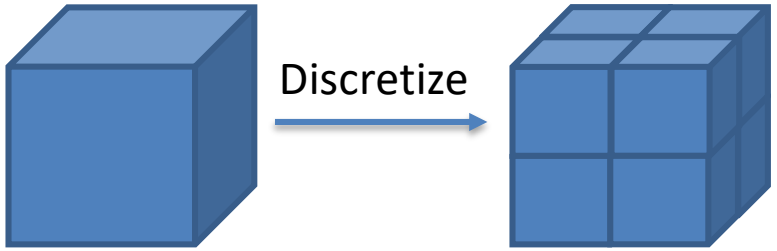
Gravitational force



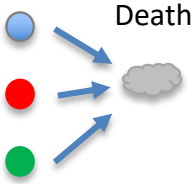
Nutrient Mass Balance

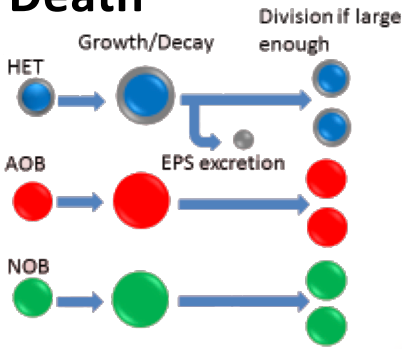


Solve using FDM

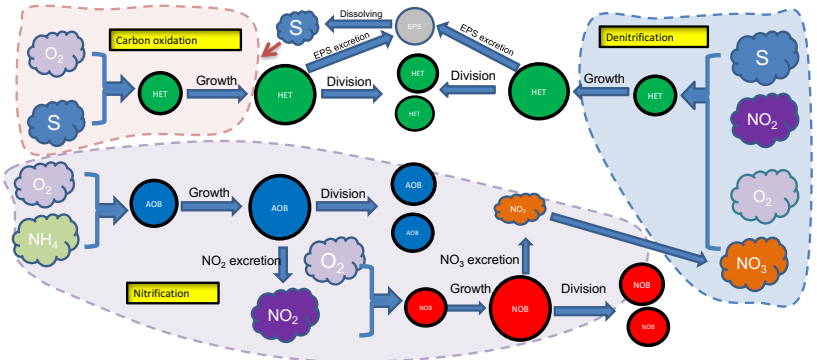


Handle Growth/Decay and Birth / Death



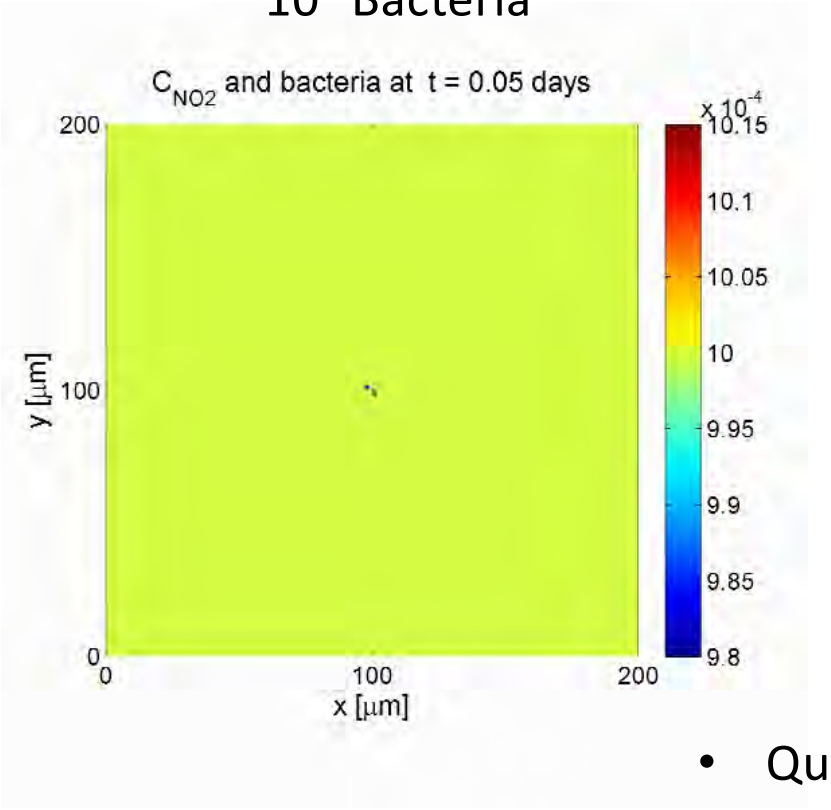


Update Growth rates wrt Nutrient



Mapping this to the Real World

10^4 Bacteria



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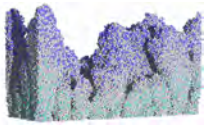
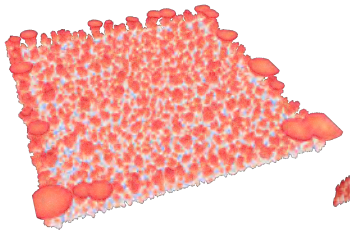
10^{18} Bacteria

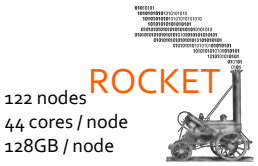
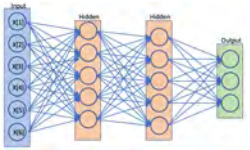
- Quality of the parameters in the model / the model
- Emergent properties as we scale up

Scaling up

frontiers in engineering biology

Under development


Volume	μm³	~100μm³	mm³	cm³	dm³
Number of Bacteria	10^4	10^6	10^8	10^{10}	10^{12+}
Simulation time	days	10's of days	100's of days	years	decades
Runtime	hours	1 day	4 days	week	week
Hardware			 122 nodes 44 cores / node 128GB / node ROCKET		
Software	MATLAB	LAMMPS	LAMMPS + MPI	LAMMPS + KOKKOS	PyTorch / TensorFlow
Purpose	Proof of concept				Emergent Properties Comparison with real world

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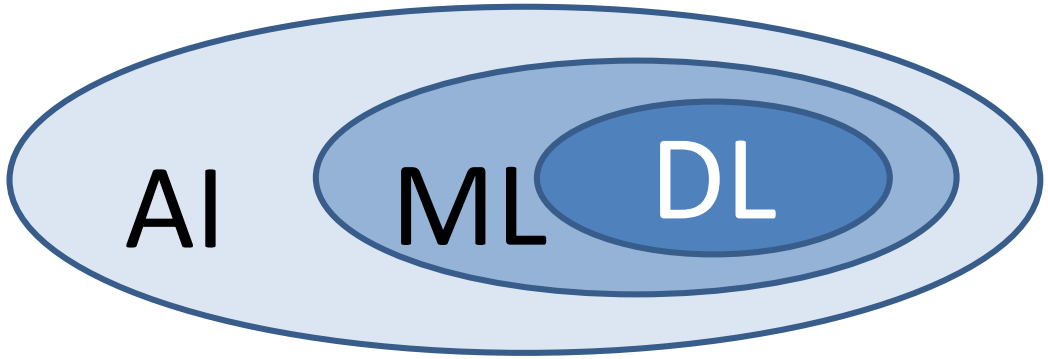
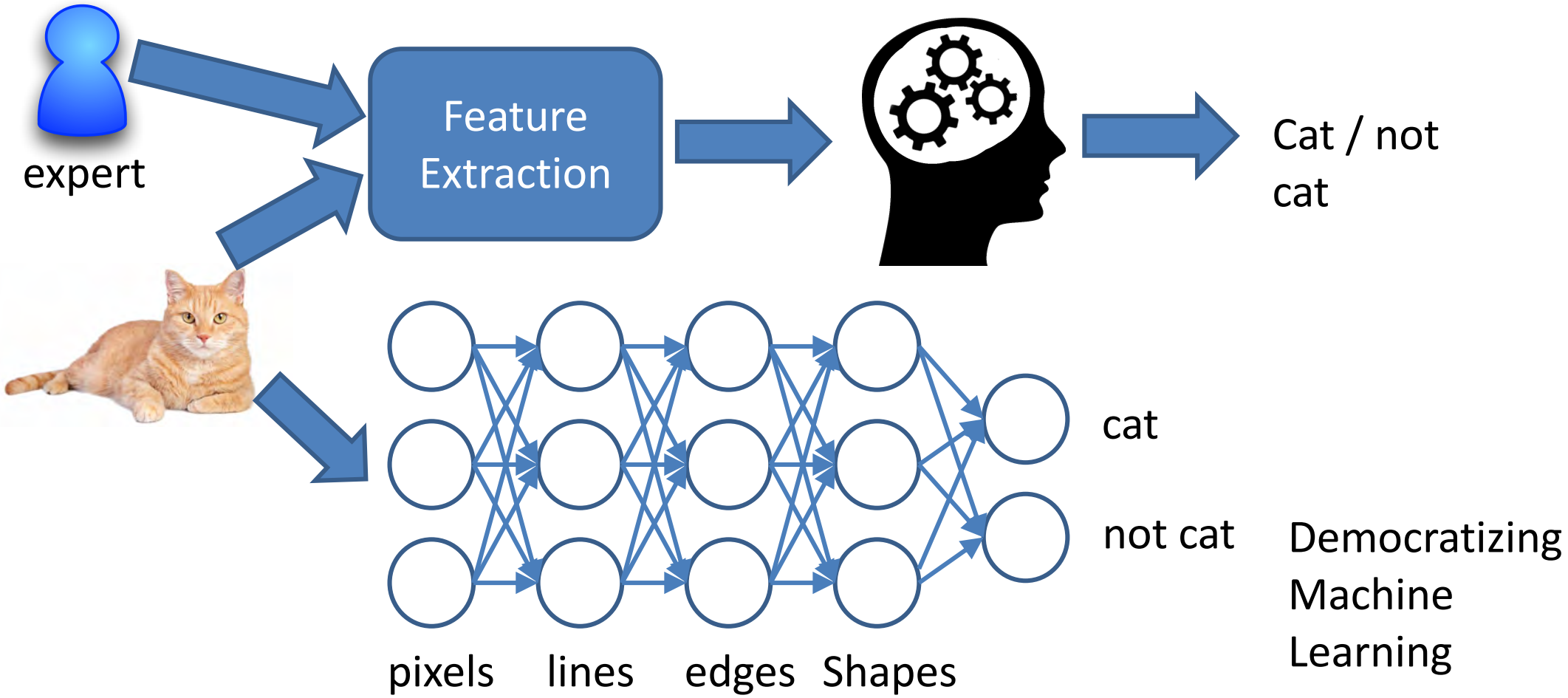
What is AI, ML and DL?

- Artificial Intelligence (AI)
  - A system which exhibits characteristics which could be seen as intelligent
- Machine Learning (ML)
  - A system which is able to learn and improve its ability
- Deep Learning (DL)
  - A system which uses (Deep) Neural Networks to exhibit ML



Machine Learning vs Deep Learning



Basic building blocks:
The data

- Data is key here: Sample as 1D array of values

X[1]

X[2]

X[3]

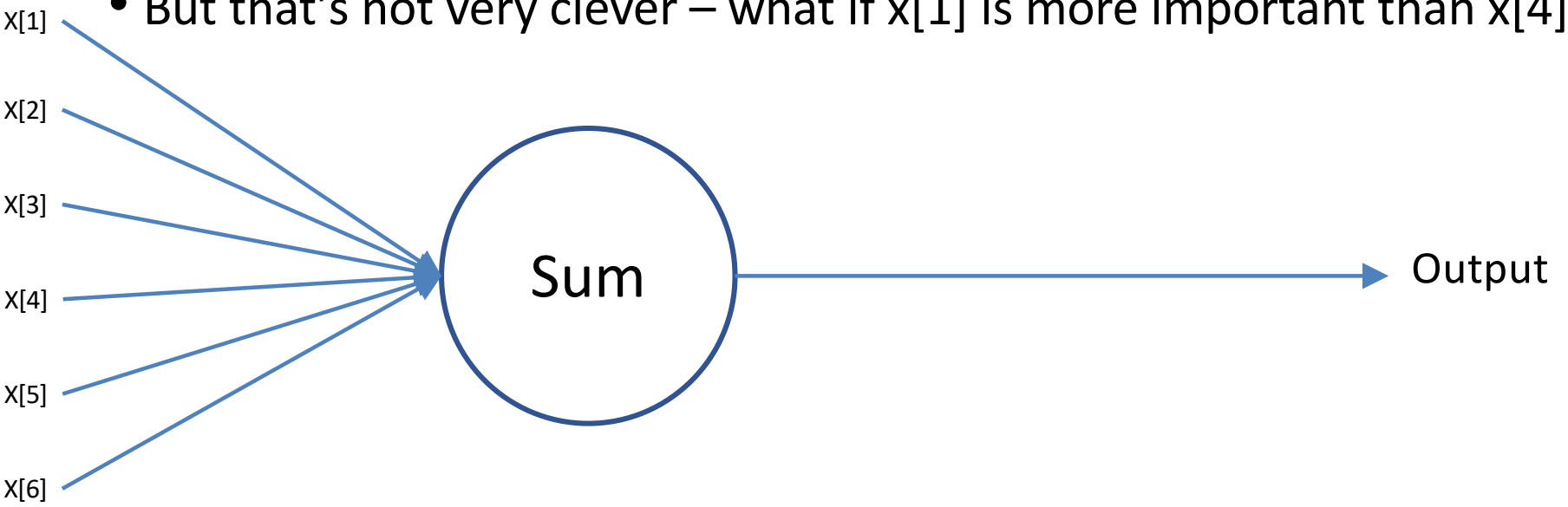
X[4]

X[5]

X[6]

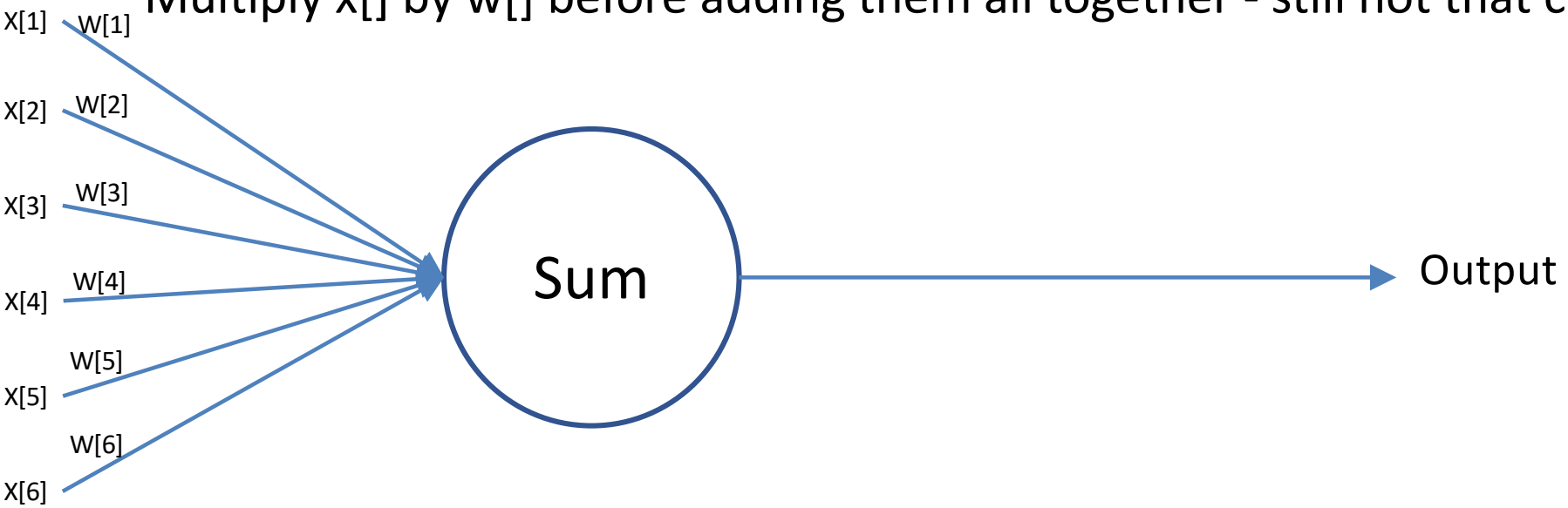
Basic building blocks: The neuron

- Sums up all of the input values
  - But that's not very clever – what if x[1] is more important than x[4]?



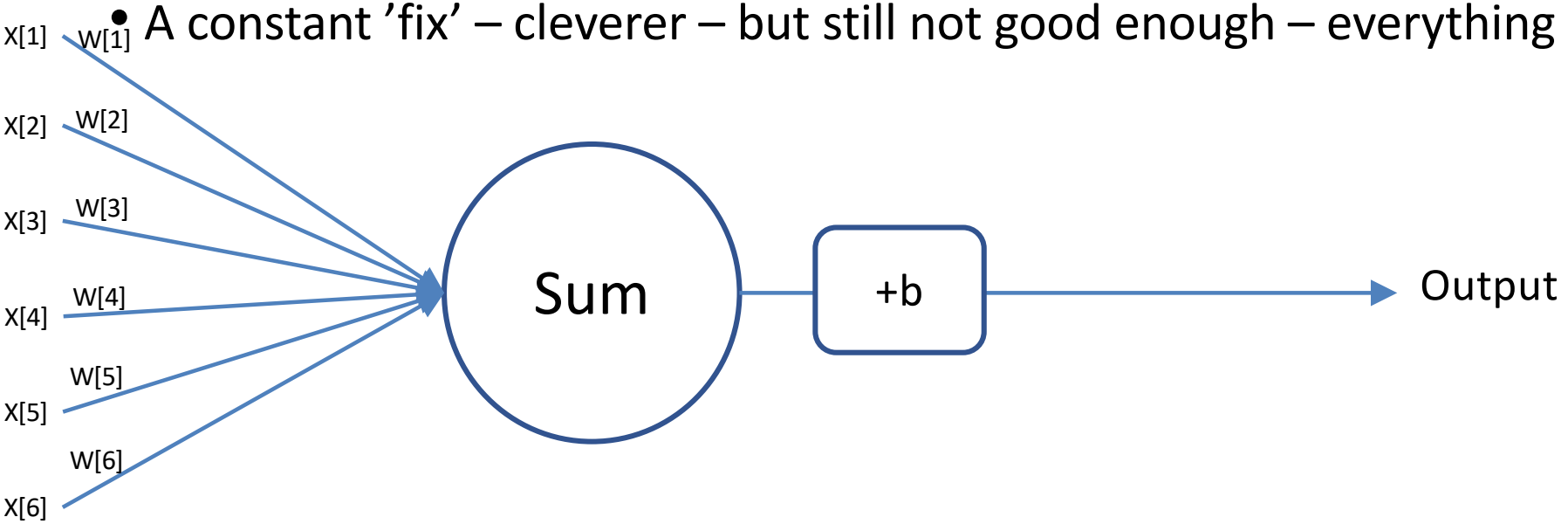
Basic building blocks: Weights

- The weights – so we can attribute importance to each x[]
  - Multiply x[] by w[] before adding them all together - still not that clever



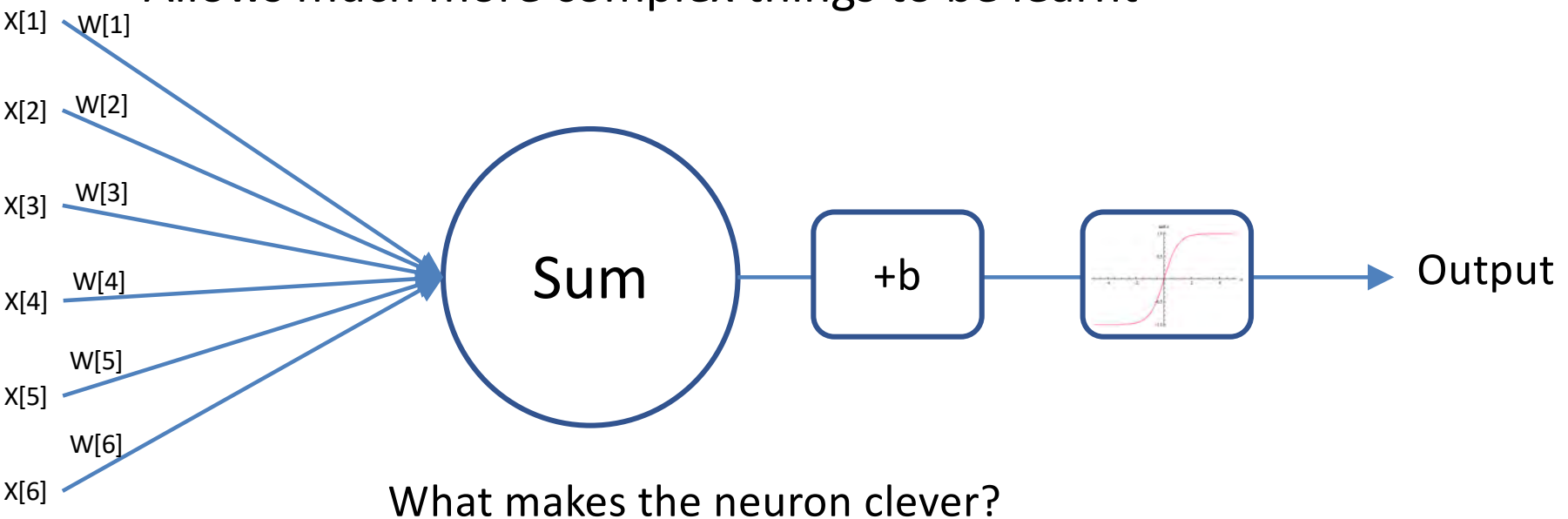
Basic building blocks:
Bias

- The bias is a value we add to the output
  - A constant ’fix’ – cleverer – but still not good enough – everything is liner



Basic building blocks: Activation function

- Activation function - non-linear operation applied to output
  - Allows much more complex things to be learnt

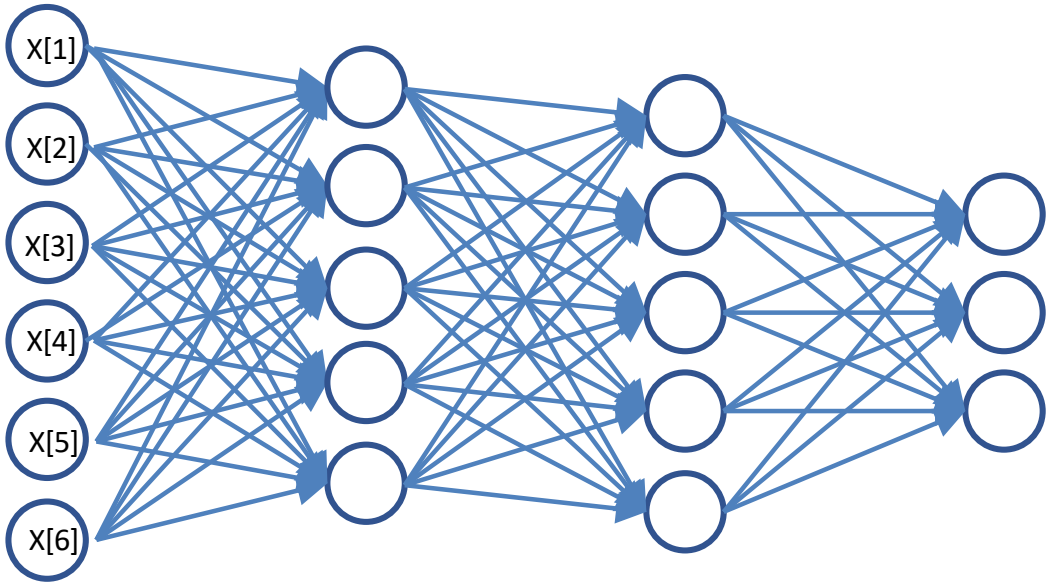


What makes the neuron clever?

- The right values of w[], b
- Trained by passing lots of examples through and modifying these values

Building a full Neural Network

- A single block on its own can’t do much
  - So, we use a whole set of them to make a neural network



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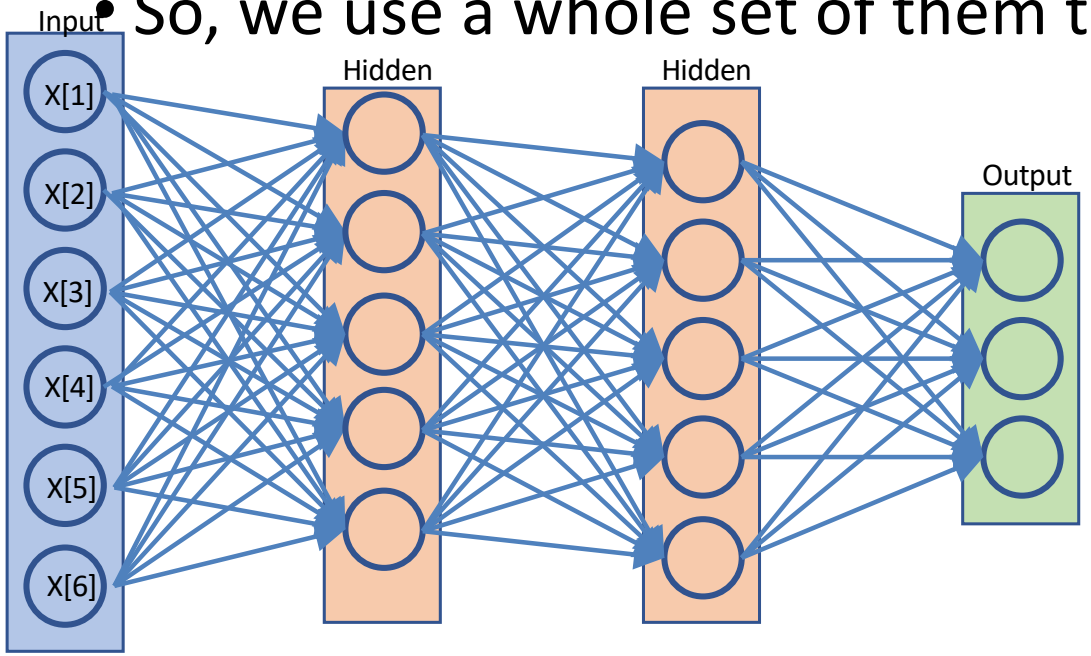

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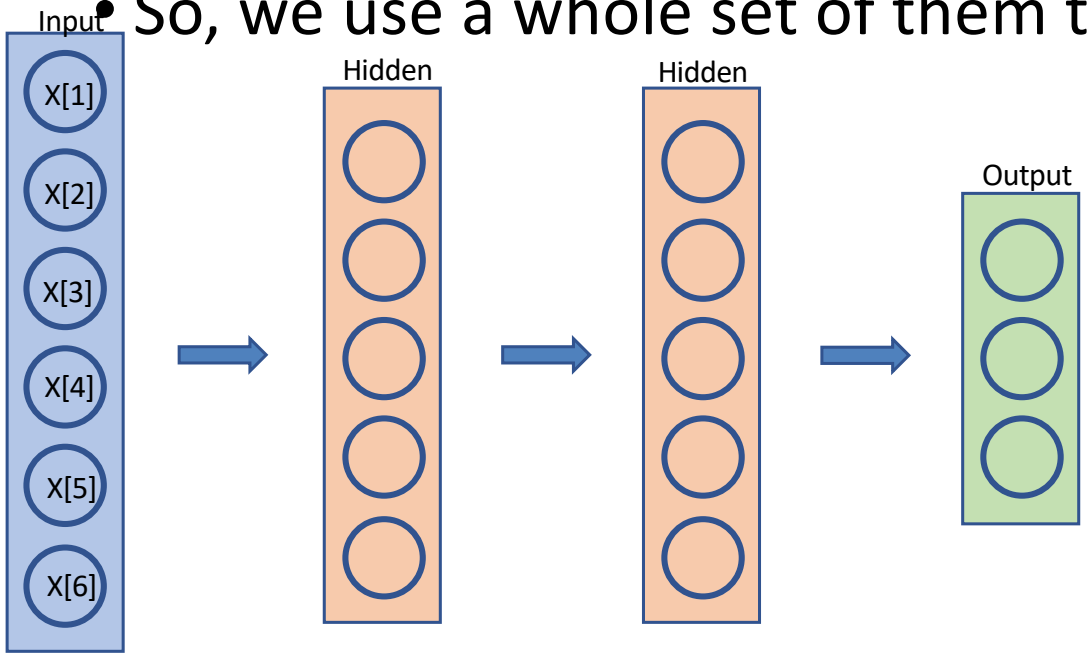

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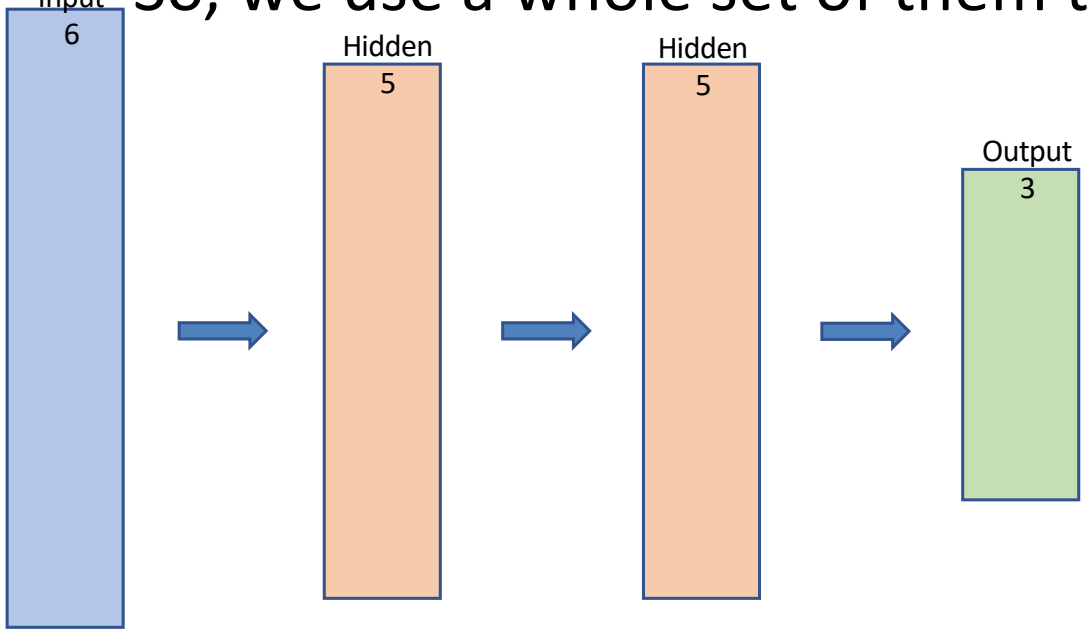
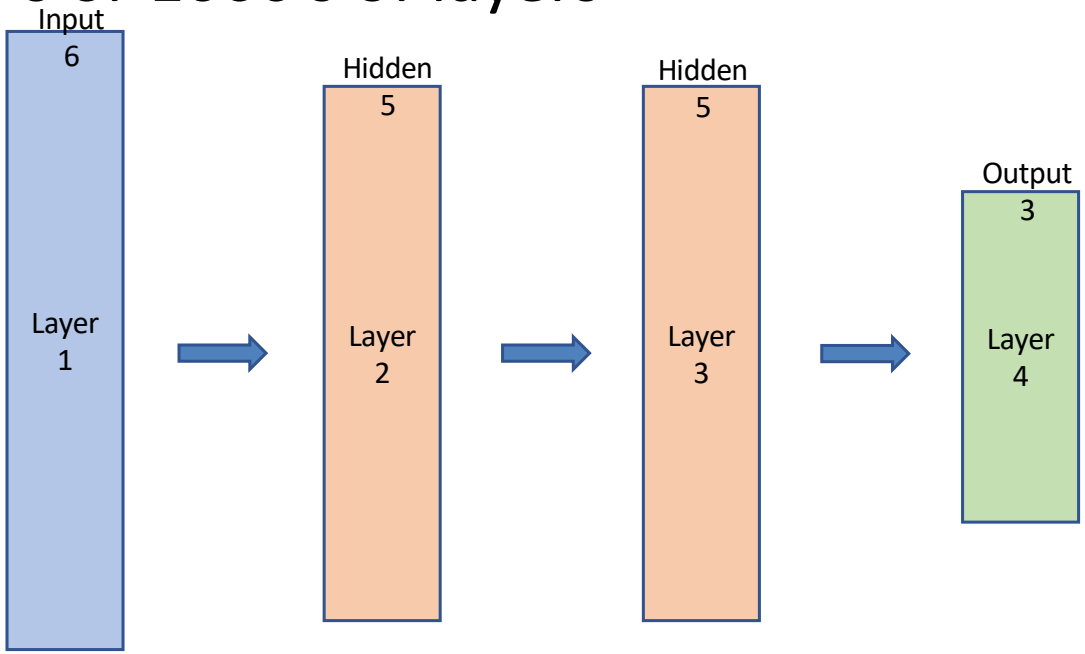


Called:

- Multi-Layer Perceptron (MLP)
- Fully Connected Layers
- Dense layers

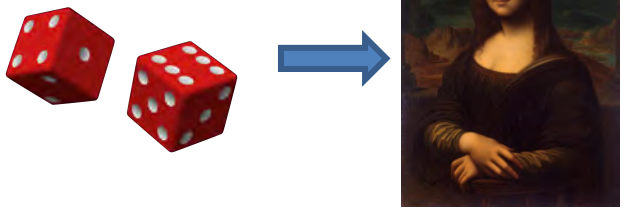
So Why Deep Learning?

- Named due to the depth of the network
- Number of layers in the network
- ‘Real’ networks have 10’s, 100’s or 1000’s of layers
- These networks are often referred to as models
- Why now?
  - Data is available
  - Powerful (GPUs) to train them



Generative Adversarial Network (GAN)

- Main aim: generate fake samples from some input domain that are as close to the real data as possible. E.g., random input -> Italian Renaissance portraits



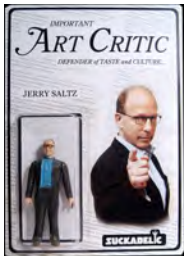
- Needs two components:

Generator

- Generates fake samples
- Tries to make the samples as 'real' as possible to fool the discriminator

Discriminator

- Identifies if a sample is fake
- Tries to identify if a sample is from the real set or a fake from the generator



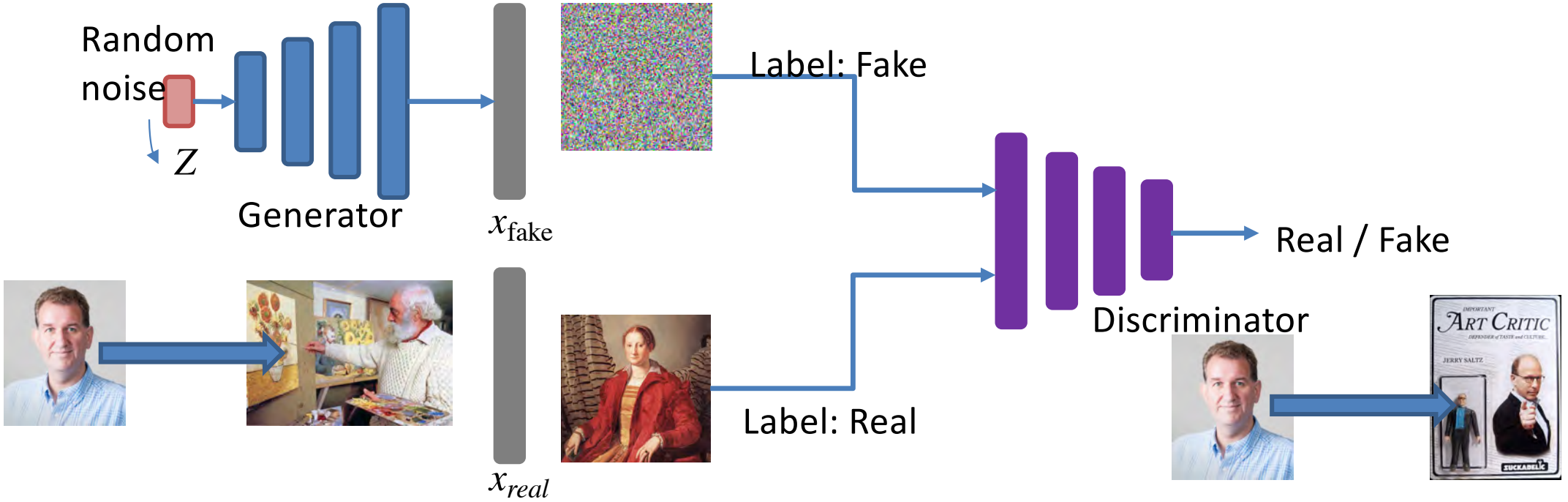
Generative Adversarial Network (GAN)

Generator

- Generates fake samples
- Forger (e.g. of art)

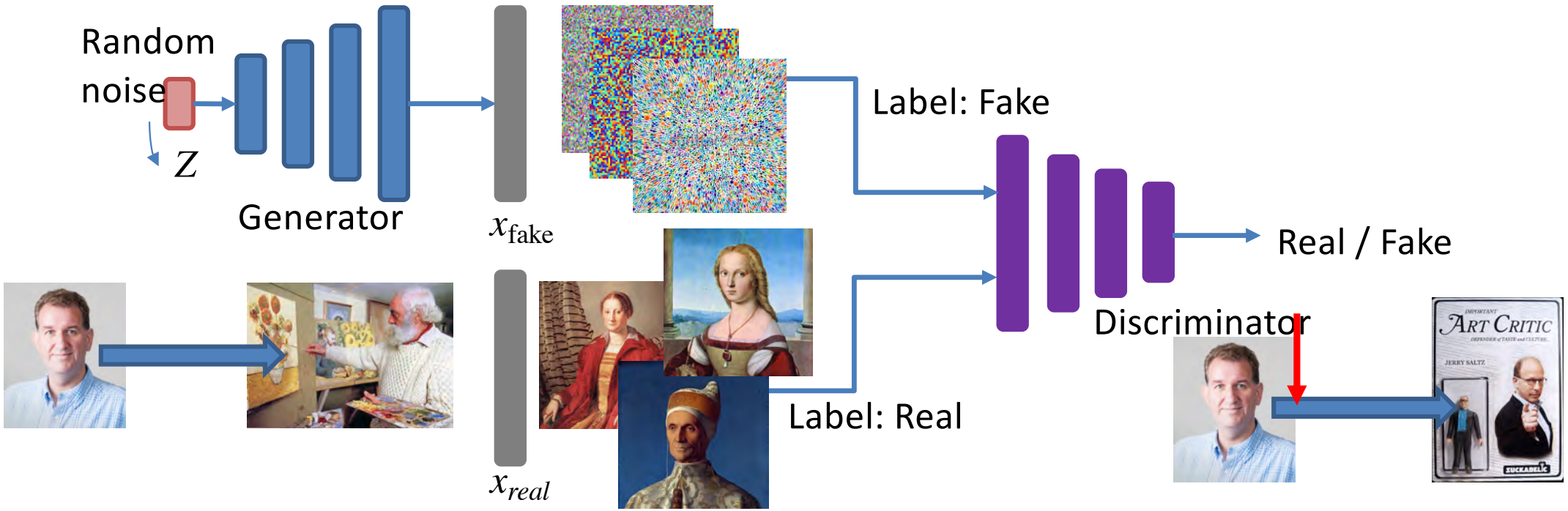
Discriminator

- Identifies if a sample is fake
- E.g., art critic



Generative Adversarial Network (GAN)

- Iteratively train **discriminator** and then generator



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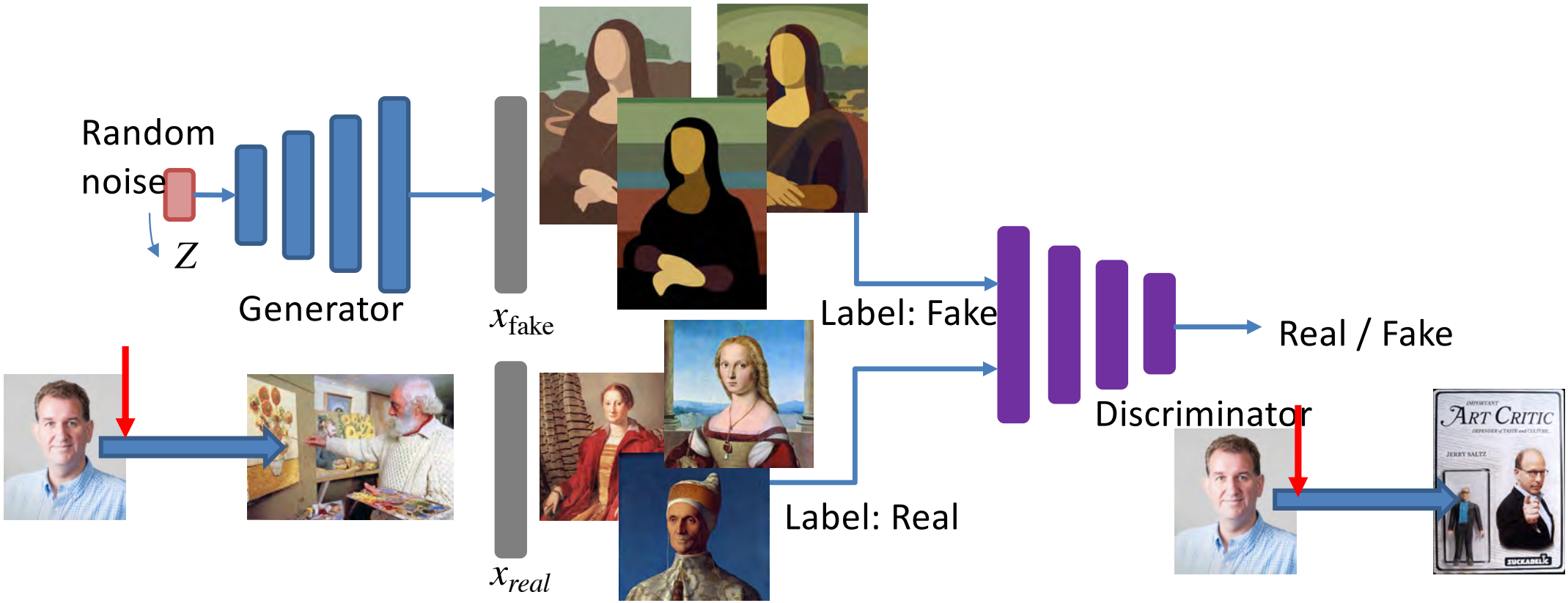

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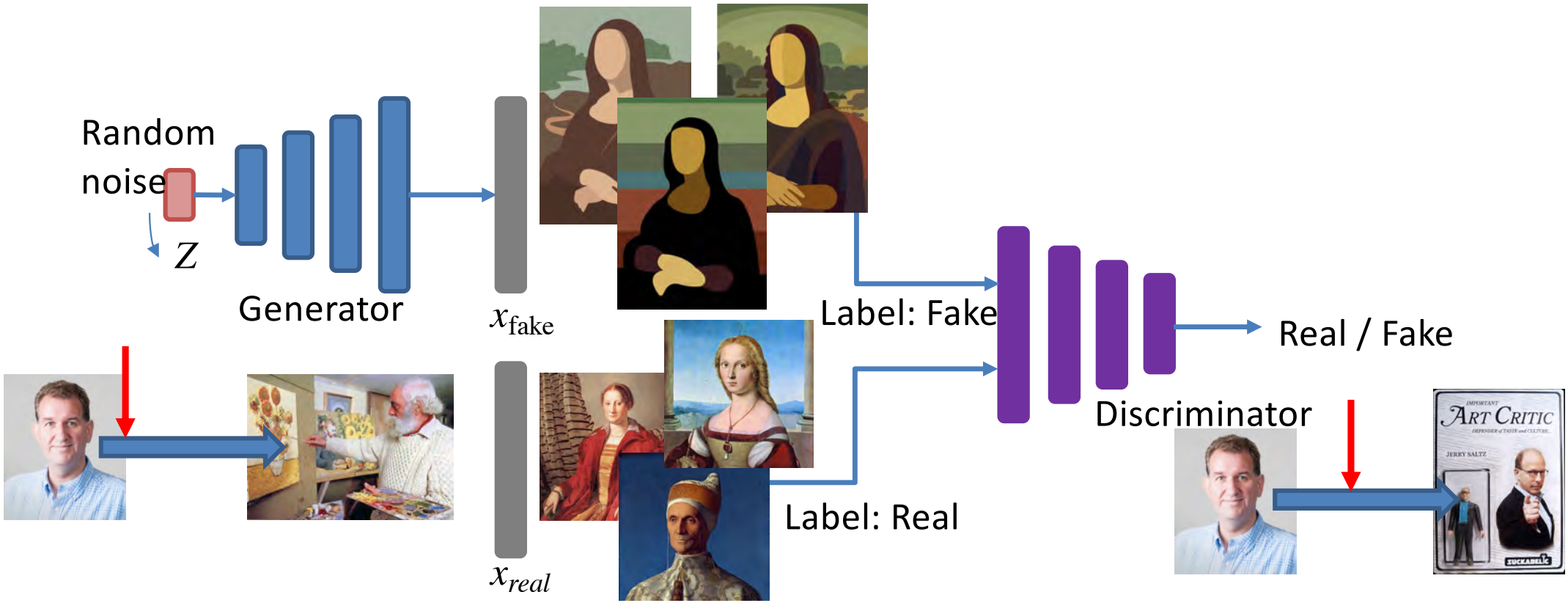

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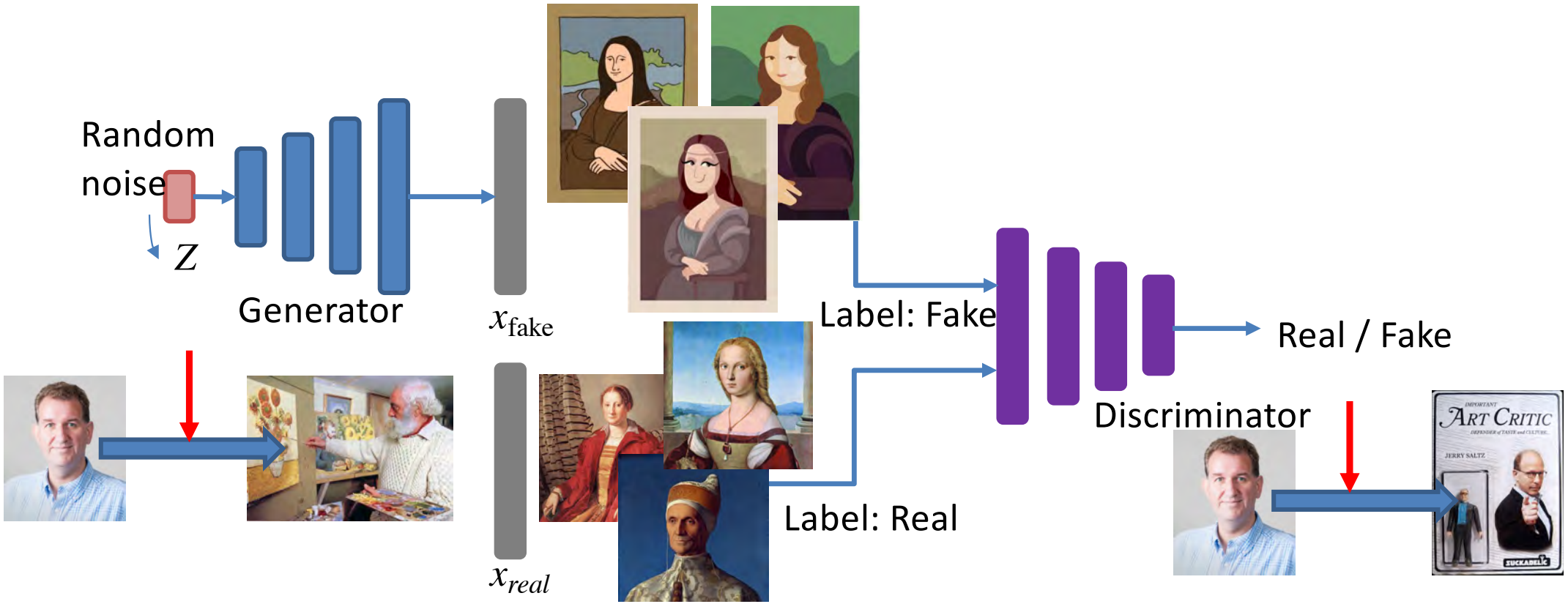

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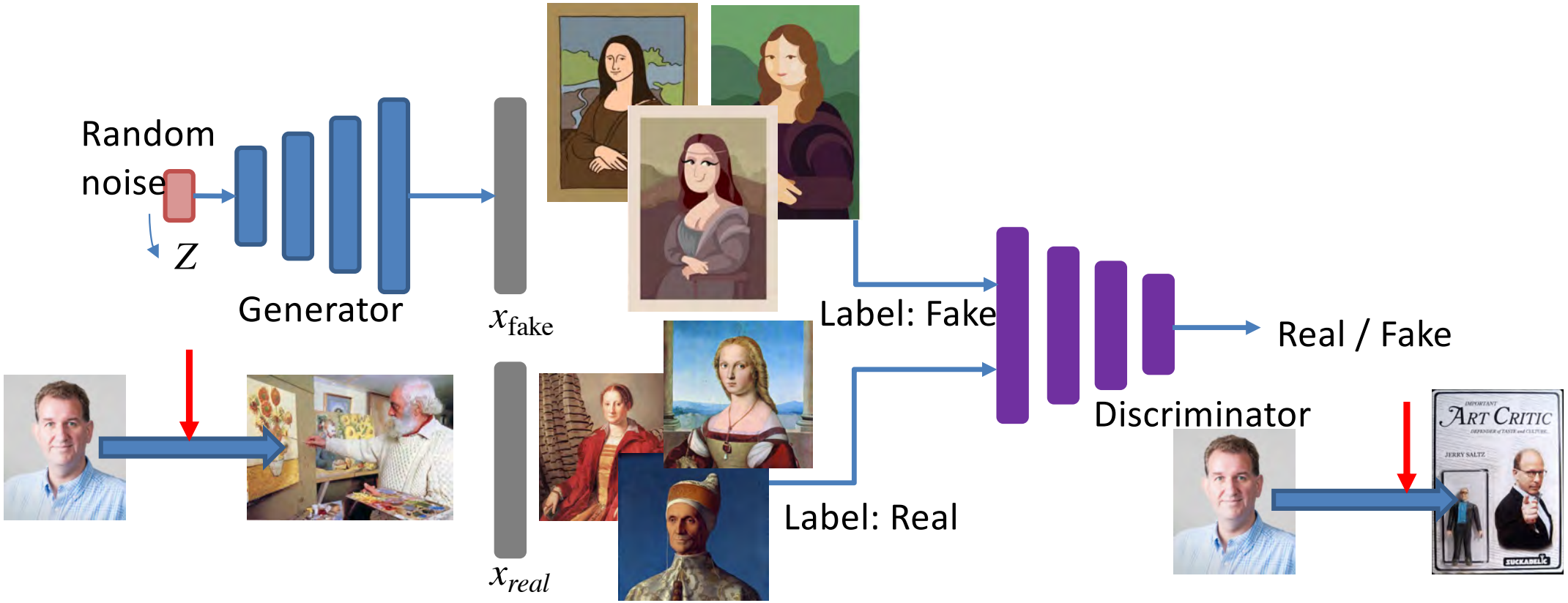

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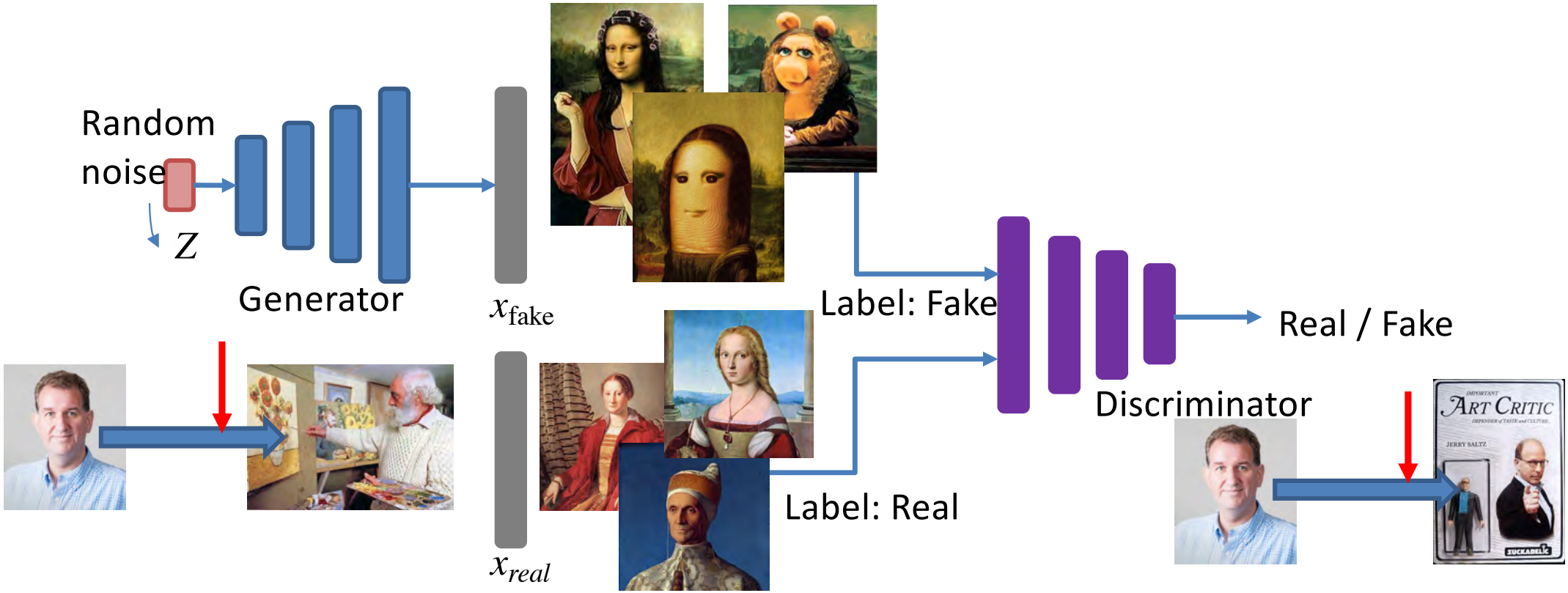
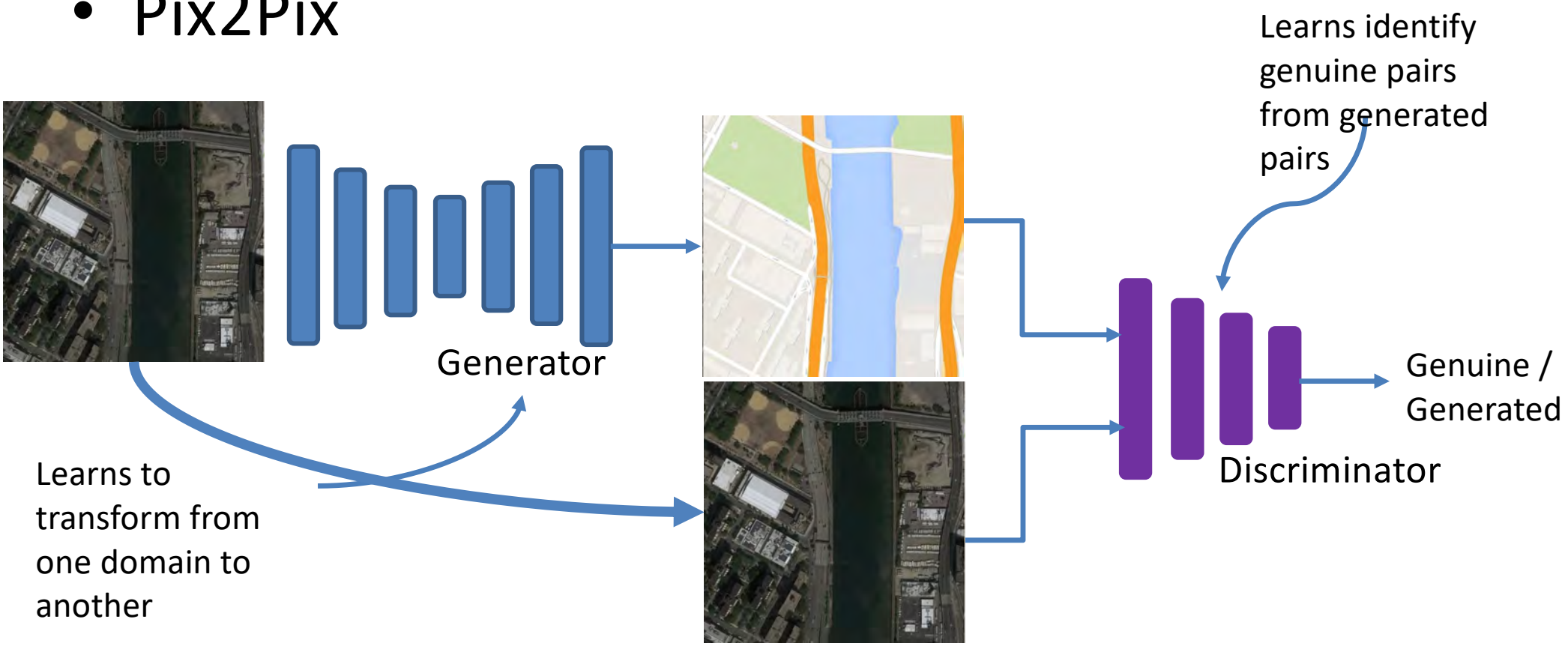


Conditional GAN

- Pix2Pix



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- **Using AI for wastewater treatment**
  - **Scaling up**
  - Fine Tuning the simulation

Building a Deep Learning Emulator

- Predict next step using Deep Learning
  - Autoencoder, GAN, RNN

  - Done for large enough volume s.t.
    sim_time >> prediction_time

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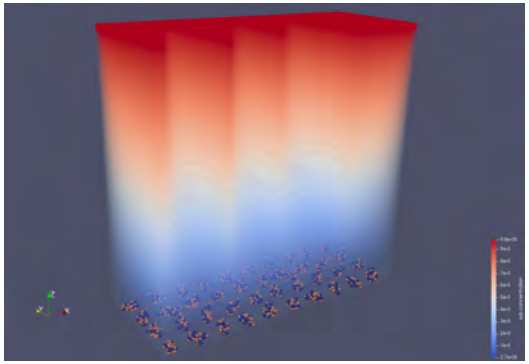

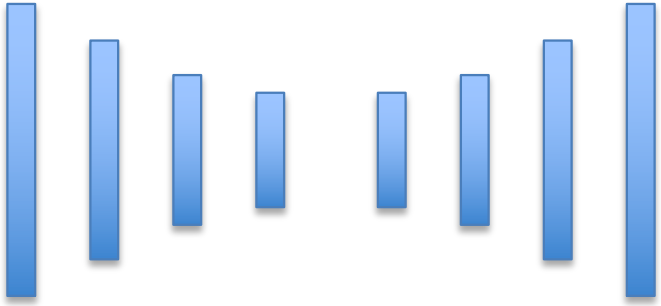

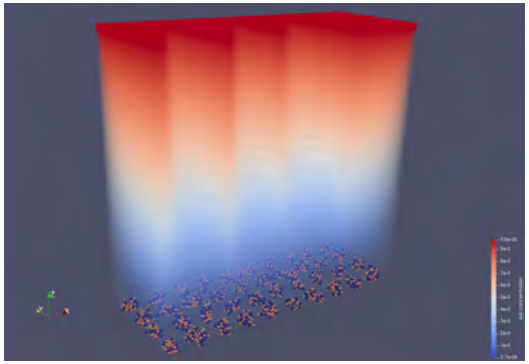

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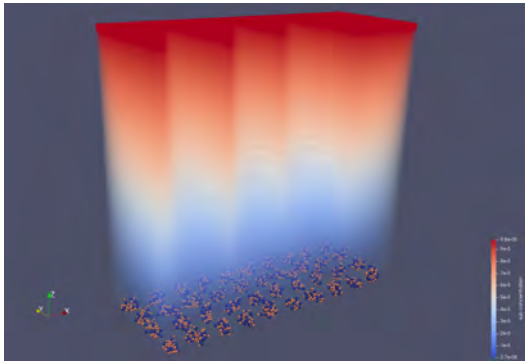
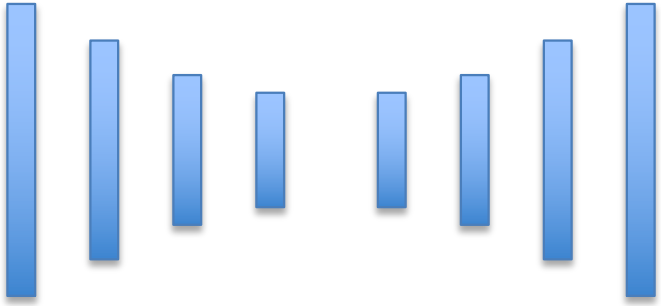
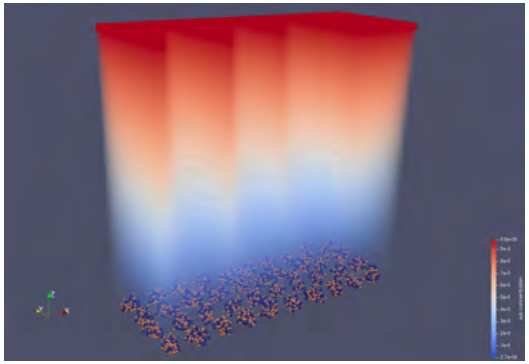

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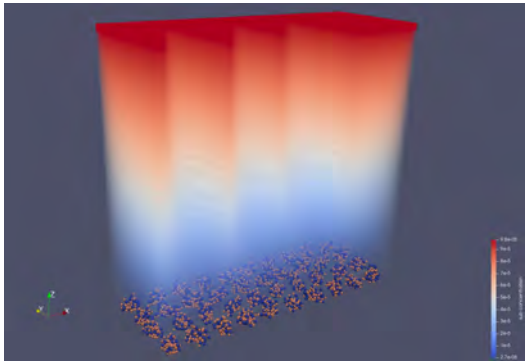
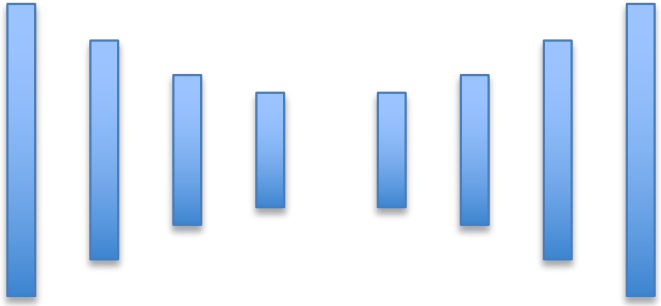
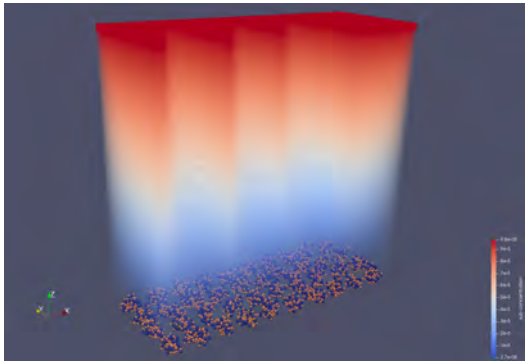

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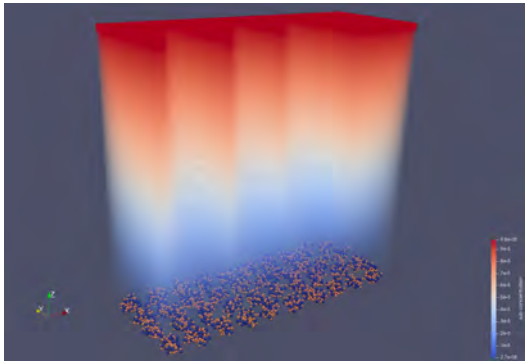
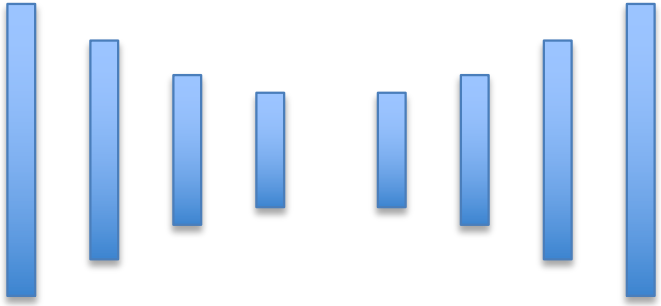
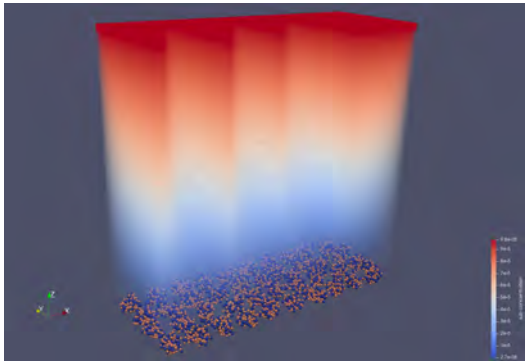
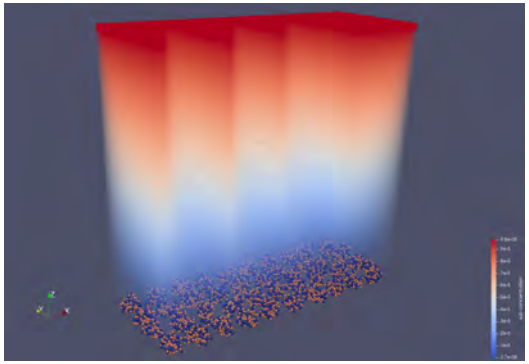
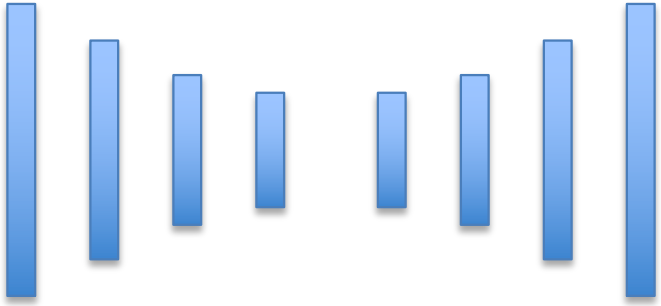
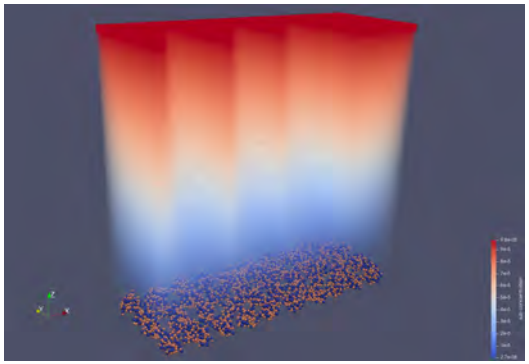




  - Done for large enough volume s.t.
    sim_time >> prediction_time

Building a Deep Learning Emulator

- Predict next step using Deep Learning
  - Autoencoder, GAN, RNN

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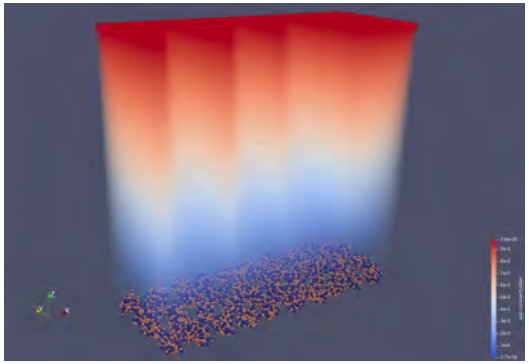
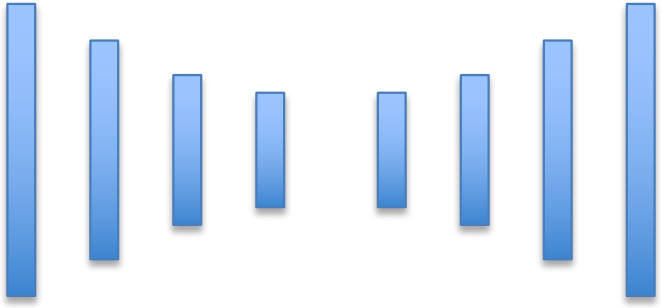
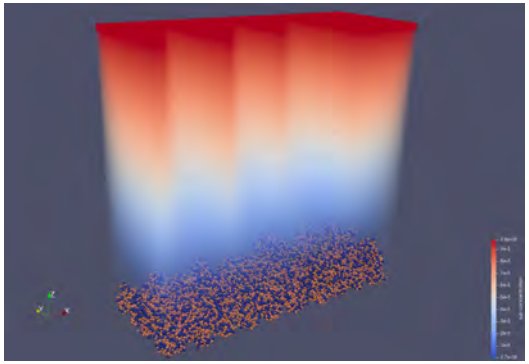

  - Done for large enough volume s.t.
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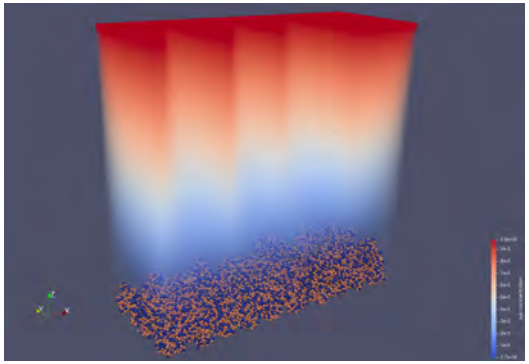
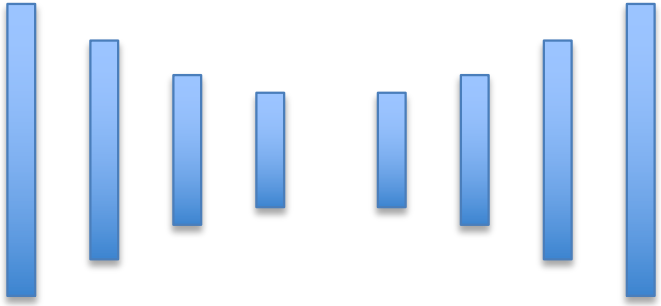
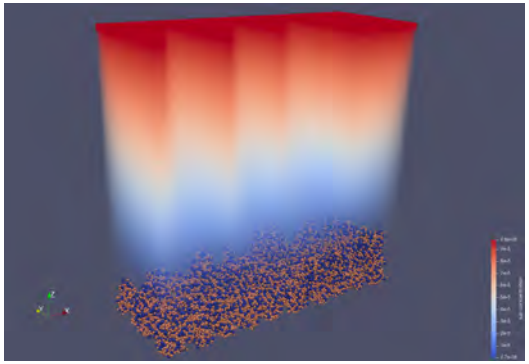
Building a Deep Learning Emulator

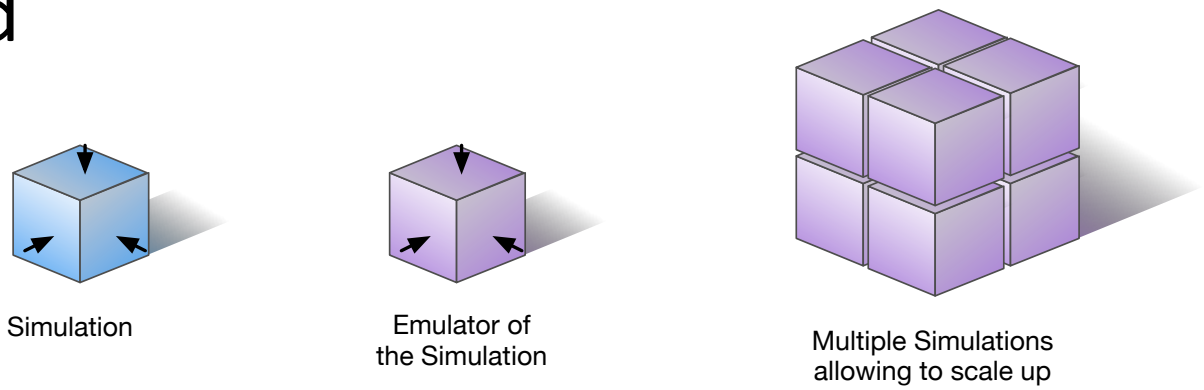
- Predict next step using Deep Learning
  - Autoencoder, GAN, RNN

  - Done for large enough volume s.t.
    sim_time >> prediction_time

How to use this to scale up

- Focus DL emulator on the Outside edges of the volume
- Can then 3D ‘tile’ volumes together
  - Nontrivial – requires massive DL Emulator, well trained



Outline

- Wastewater Treatment Primer
- Simulating wastewater treatment
- AI Primer
- **Using AI for wastewater treatment**
  - Scaling up
  - **Fine Tuning the simulation**

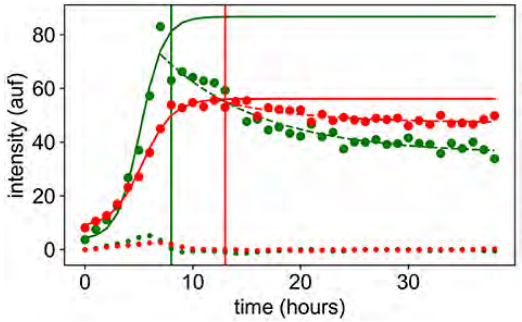
Why might the simulation need tuning?

- Simulations are ‘best guesses’ as to how a system works
  - Parameters often based on results from papers/ books
  - Model is based on our understanding of how the system works (often from books)
  - Can we match the output of the simulation to the real world?

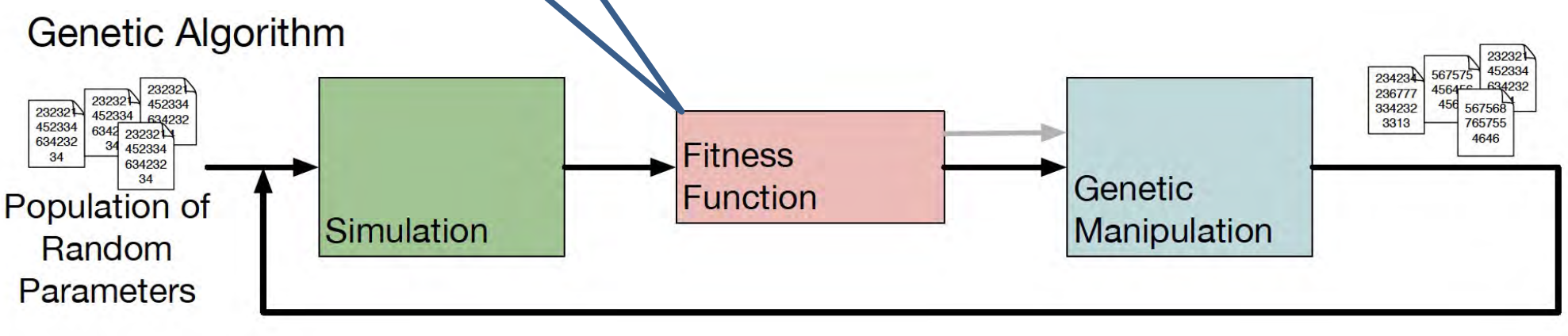
Start with a fairly simple Genetic Algorithm approach

$$\frac{A}{1 + e^{(\frac{4\mu}{A}(\tau - t) + 2)}}$$

A, μ and τ



Genetic Algorithm



Hand-Crafted Fitness

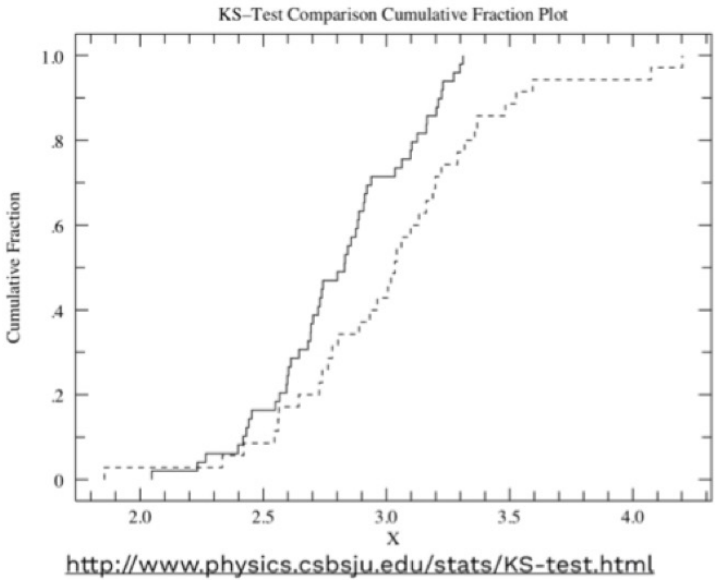
- Fitness function defined by comparing experimental and simulation data
- Multiple runs of simulation
- From each simulation compute A, μ and τ
- Compute empirical CDFs
- Compare with same for experiments

Let F and G be empirical CSFs for simulation / experiment data

$$L(F,G) = \int_{-\infty}^{\infty} |F(x) - G(x)|\, dx$$

To obtain a fitness function f from a loss L

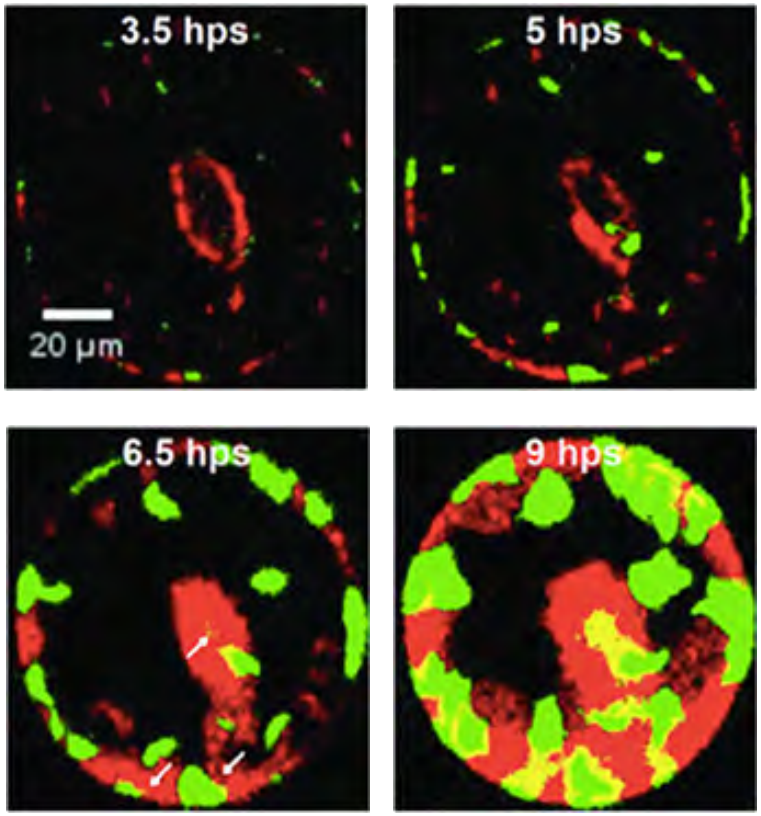
$$f = \frac{1}{0.1 + L}$$



http://www.physics.csbsju.edu/stats/KS-test.html

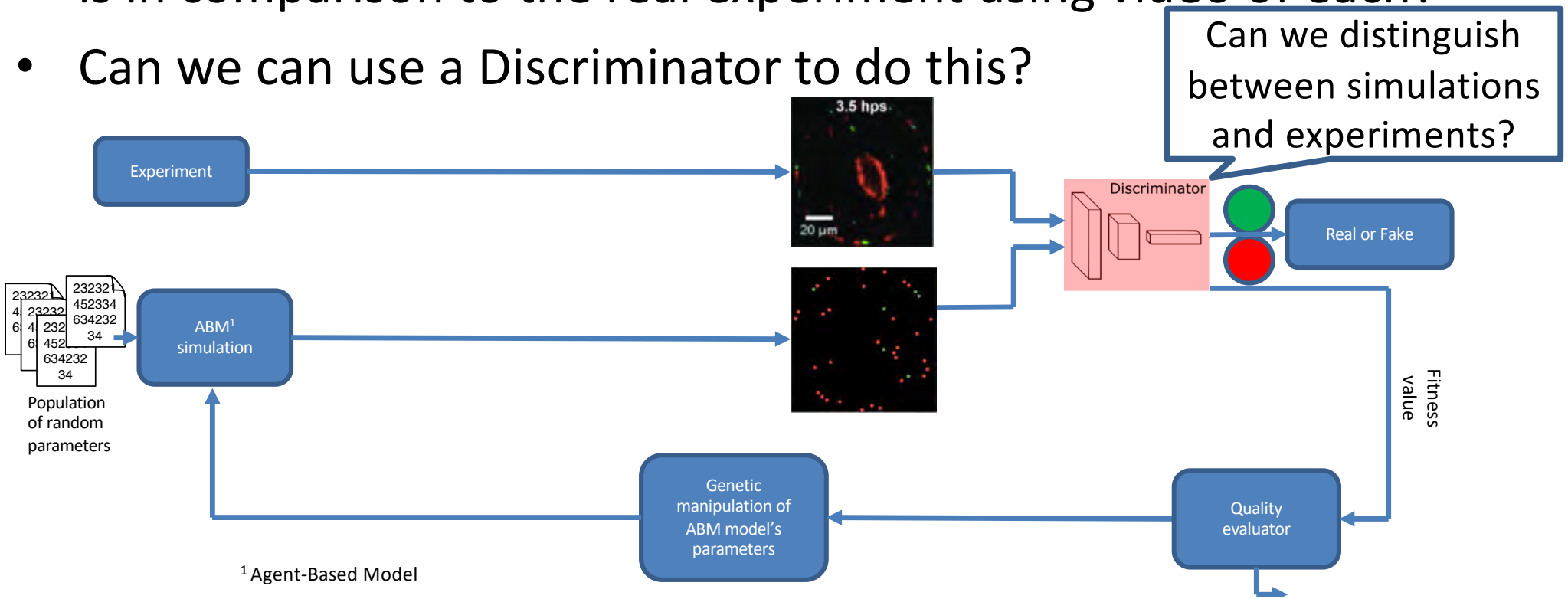
Brain storm – what else is there?

- The number of regions of each bacteria
- Their shape
- Their relative locations
- Are they touching?
- How these things change over time
- …



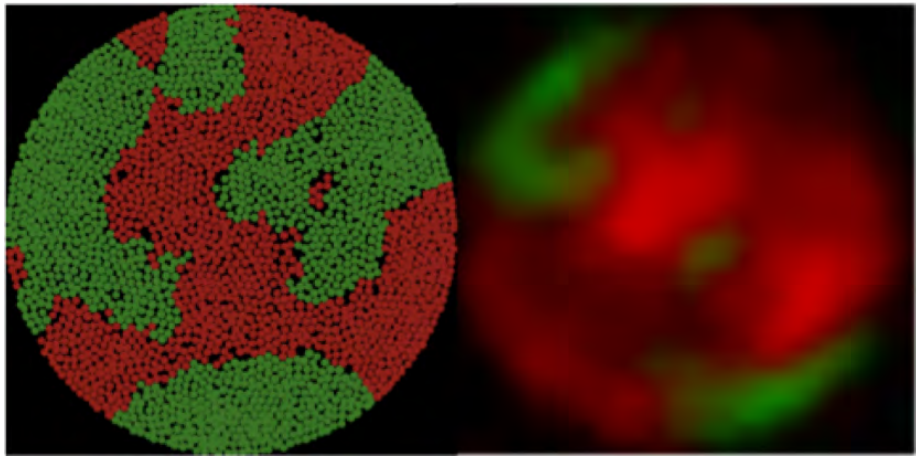
Deep Learning says ‘don’t do feature extraction’

- Can we get Deep Learning to tell us how good our simulation is in comparison to the real experiment using video of each?
- Can we can use a Discriminator to do this?



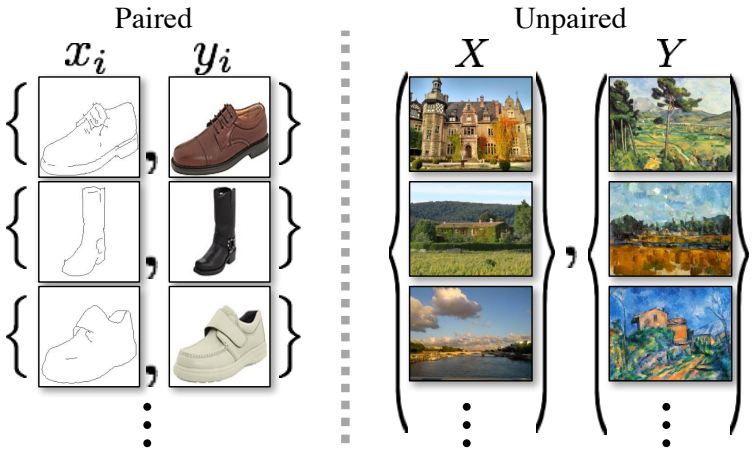
This will fail: Simulation looks nothing like Experiment

- Simulation is nice crisp and clean
- Fluorescence of tightly packed bacteria

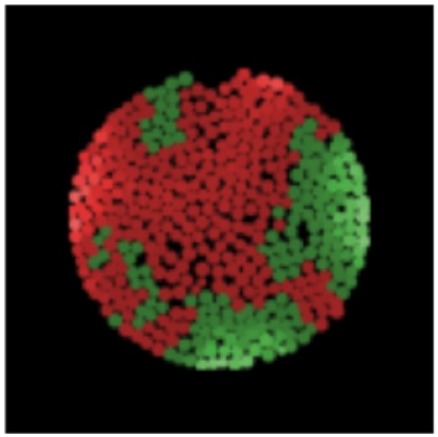


Making Simulations look more 'Real'

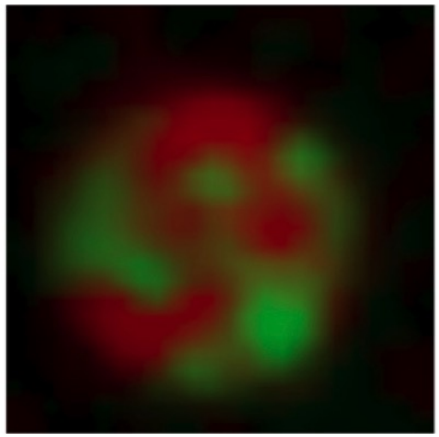
- Style Transfer
- Using CycleGAN
- No need for paired images



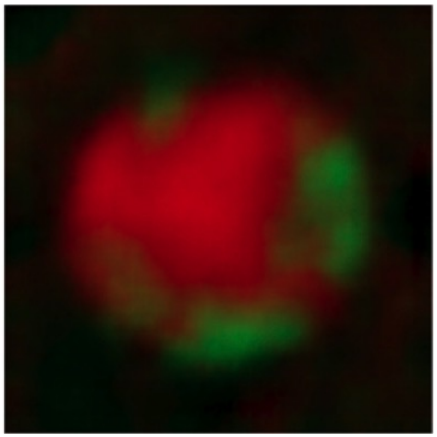
Input (simulation)



Source (experiment)

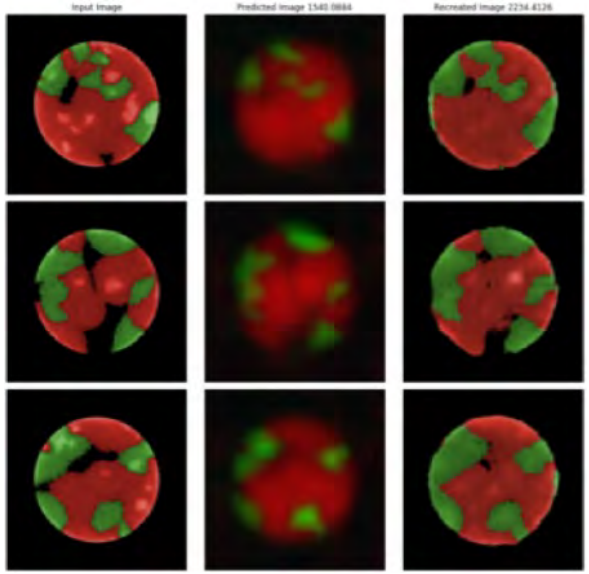


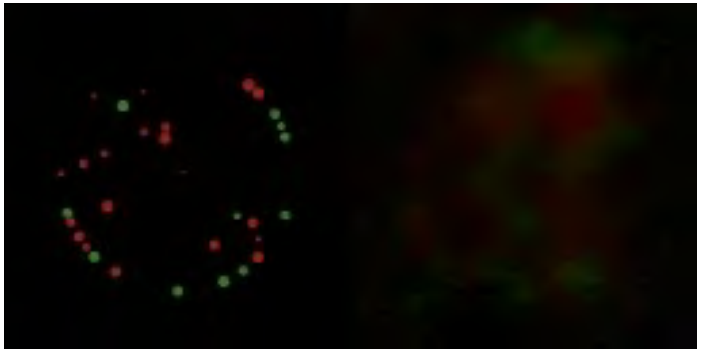
Output (experiment-like sim)



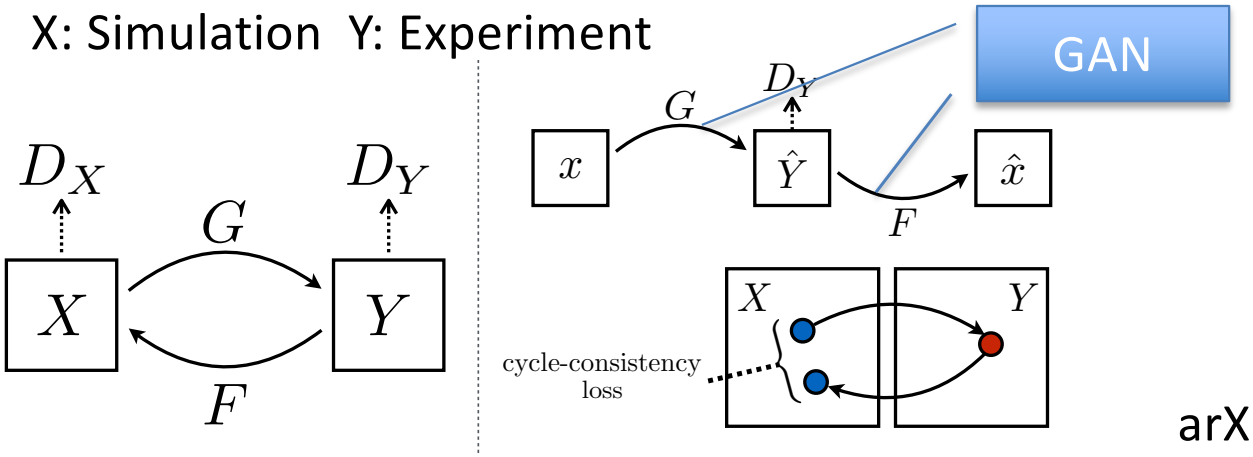
Style transfer of simulation data

- Unpaired Image-to-Image Translation
  - CycleGAN
- Pre-trained on images that resemble the distribution of the experiments
- Pad images to match size of experiment



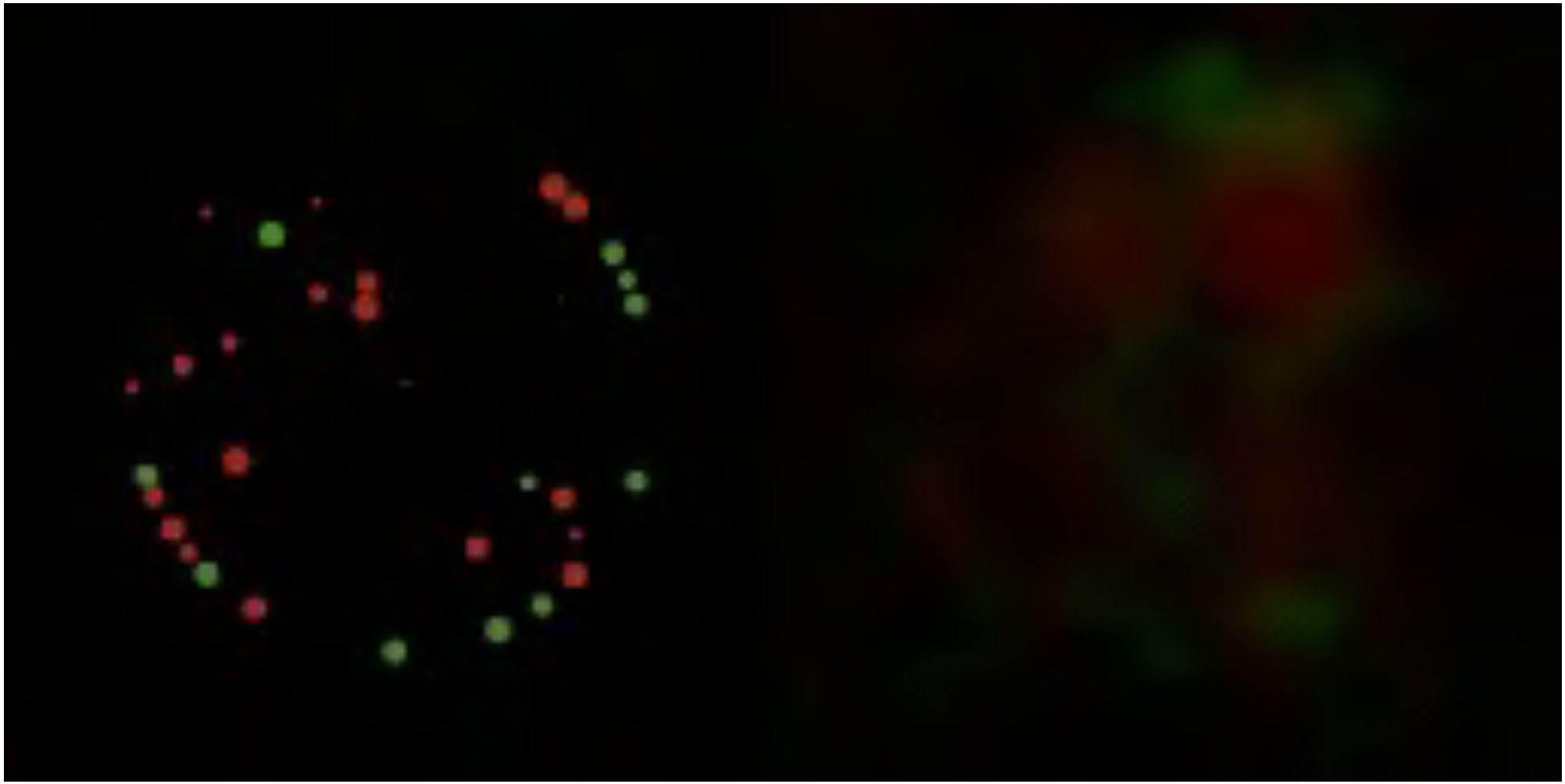


X: Simulation Y: Experiment

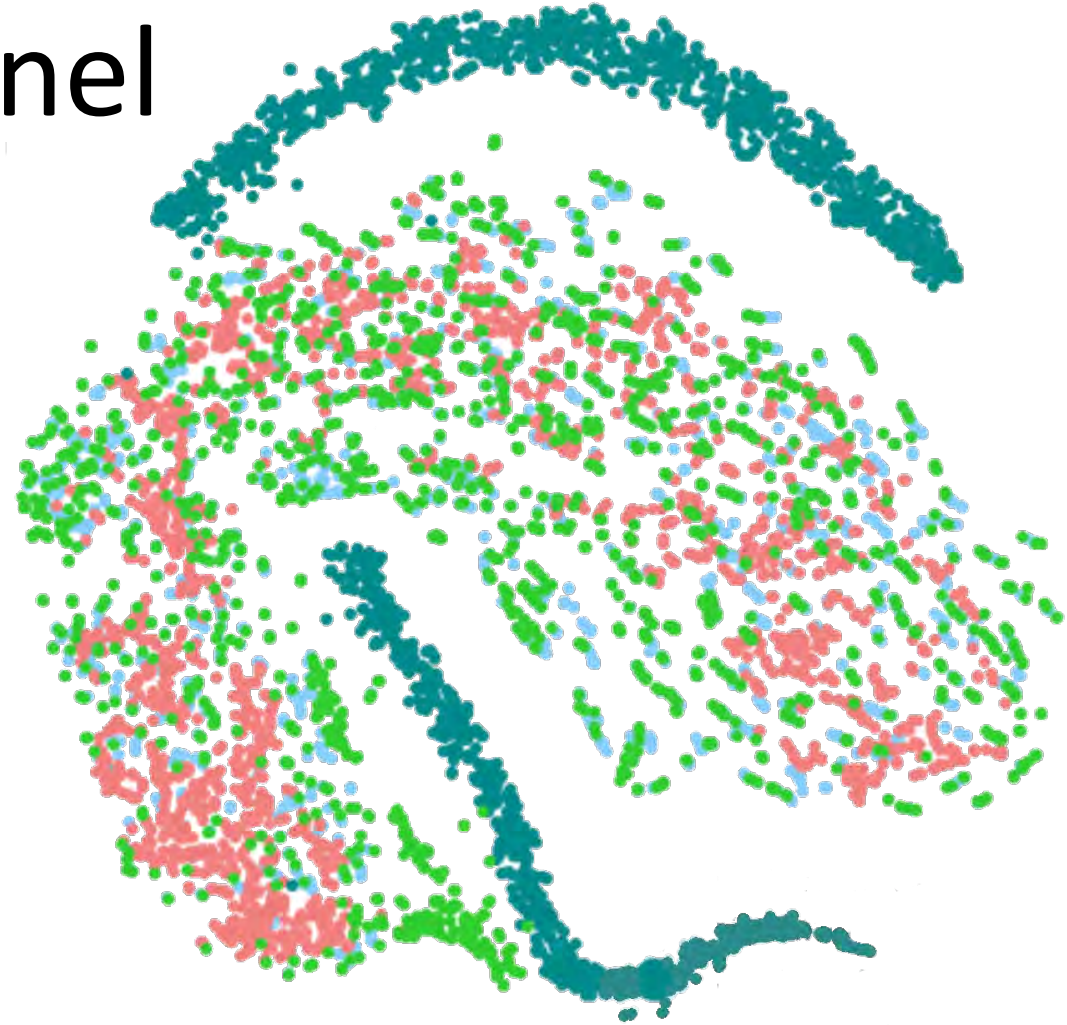


arXiv:1703.10593v6 [cs.CV] 15 Nov 2018

The finished simulation



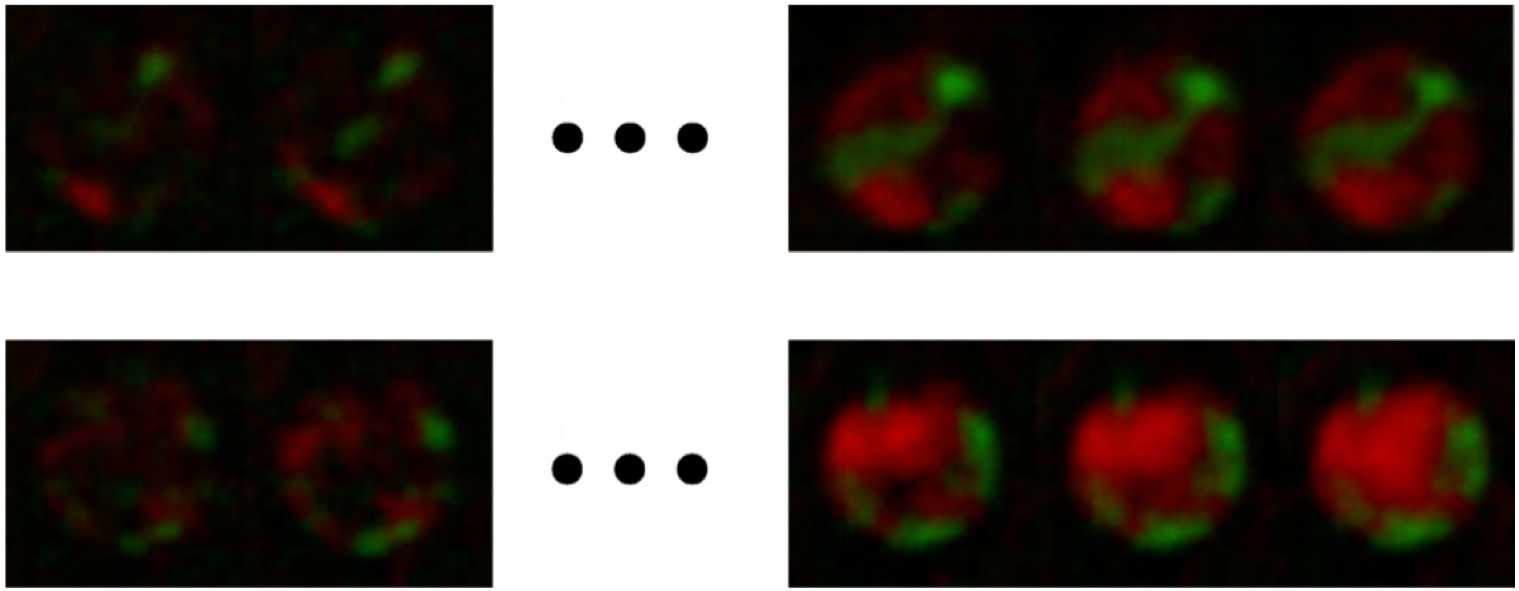
T-SNE Liner Kernel



- Experiment
- Experiment Artifact
- Simulation
- Simulation Style Transfer

Discriminator

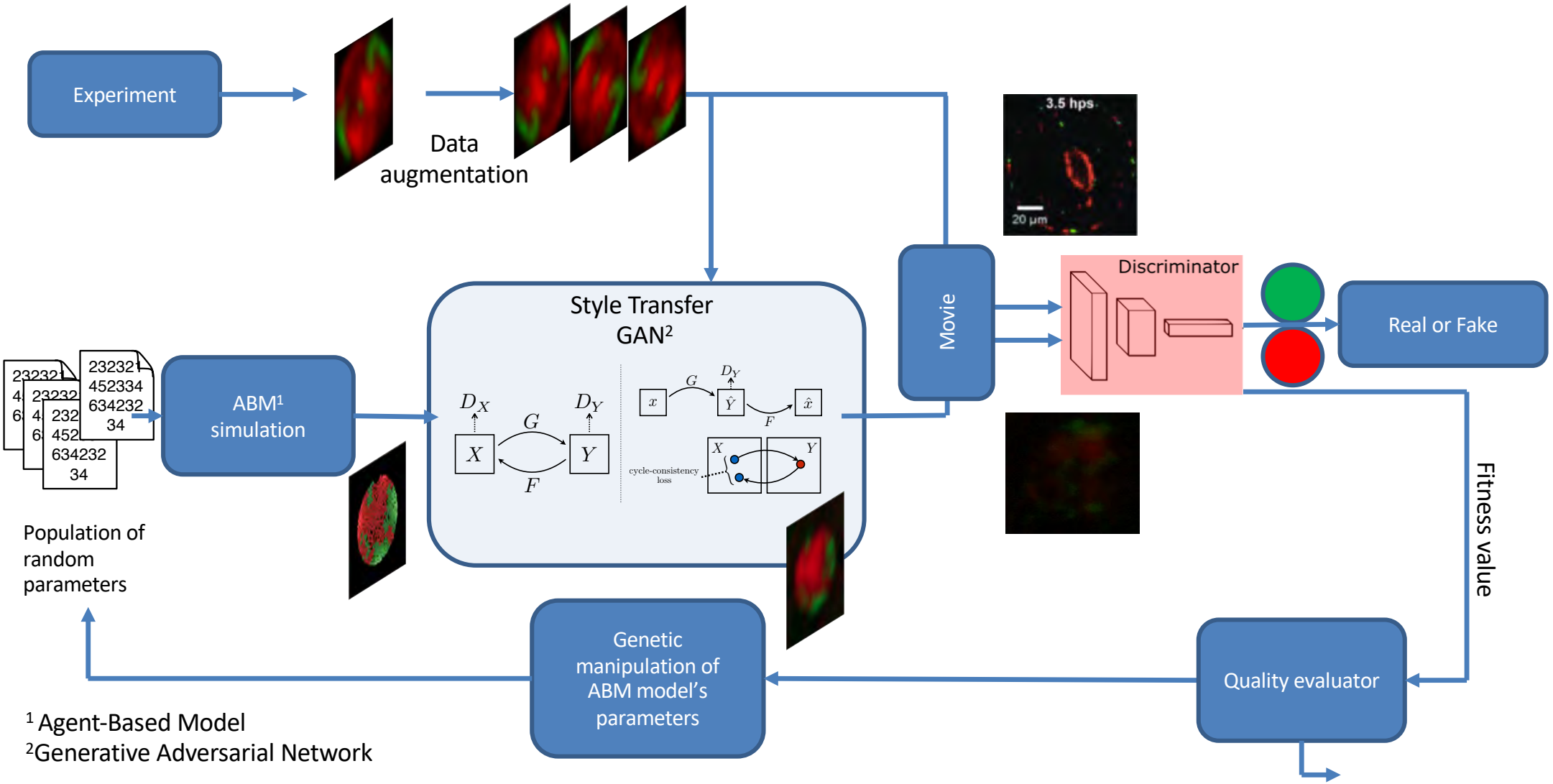
Input: 15 images of the growth phase



Experiment

Simulation

AI Framework for Creating Accurate Agent-Based Models of Microbial Populations



[1] Agent-Based Model
[2] Generative Adversarial Network

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Summary

- To make better simulations we need:
  - Larger Scale -> observe emergent properties
  - More accurate simulations -> fine-tune
- Larger simulations
  - Scale up with emulators
- More accurate simulations
  - Tune parameters / agents to experiments

Many thanks to: Denis Taniguchi, Miguel Fuentes-Cabrera, Daniel Elbrecht, Gavin Glenn, Ryn Gray, Grace Kim, Austin Li, Lino Valdovinos and the NUFEB team

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