



# AI FOR SCIENCE SUMMIT

DAY 1: 25/11/24

## A MORE DYNAMIC VIEW of DEEP LEARNING

WITH THE EMERGENCE OF...

- DRUG DISCOVERY: GENERATING MOLECULES
- CATALYSIS: ACCELERATE REACTIONS
- MATERIAL SCIENCES
- AND MORE! (GENAI, ALPHAFOLD)

SOMETHING IS SHIFTING IN SCIENCE

AI DISRUPTION IN 2 STEPS:

- FROM EXPERIMENT to COMPUTER SIMULATION
- AM OR TIZE
- FROM SIMULATION to EMULATION

GOALS of DEEP LEARNING

- BUILD ABSTRACTIONS
- REASONING
- ADVERSARIAL ROBUSTNESS
- UNCERTAINTY CALIBRATION

WE NEED A MORE DYNAMIC VIEW of ML:

- ML IS the NEW HAMMER for...
- OSCILLATORS
- TRAVELLING WAVES
- SYNCHRONISATION

COMPUTATIONAL SCIENTISTS

USE of EXPLAINABLE ML MODELS IN METABOLIC MEDICINE

- SUPERVISED learning MODELS to PREDICT BMI
- RANDOM FOREST MODEL to IDENTIFY IMPORTANT FACTORS IN OBESITY
- CLEAR EXPLAINABLE MODELS & VISUALISATIONS

RECURRENT VAE with GAUSSIAN PROCESS DECODERS

WE NEED to FIND the BEST WAY to REPRESENT MOLECULES SO THAT THEY'RE MACHINE READABLE

E.G. MOLECULAR PROPERTY LANDSCAPE

Unravelling the string theory landscape

WE DON'T KNOW the DEFINITION of STRING THEORY

USE ML to APPROXIMATE this GEOMETRIC LANDSCAPE!

DISCOVERING ELECTROCHEMISTRY with ELECTROCHEMISTRY-INFORMED NEURAL NETWORKS

ECINN

BIG DATA IS NOT the ONLY DATA for ML

USE ELECTRO-CHEMICAL PRINCIPLES to INFORM OUR NEURAL NETWORK

TITLE: FIRST STEPS USING TOPOGRAPHIC DEEP NEURAL NETWORK MODELS IN the VENTRAL STREAM

NEURAL NETWORKS CAN PREDICT NOVEL BRAIN REGION SPECIALISATION VIA TOPOGRAPHIC CLUSTERING

PARTNER: PERSON

BIKE

APPLICATION of AI/ML

RL AUTONOMOUS CONTROL COULD HELP ACHIEVE THIS!

micro REACTORS ARE THE AIM FOR NUCLEAR POWER

IN NUCLEAR

THERE IS NO LIMIT to HOW MUCH ENERGY NUCLEAR FISSION CAN CREATE

CONTROL is NEEDED!

DISENTANGLLED MULTIMODAL REPRESENTATION MODELS IN HEALTHCARE

ECG TEST

MRI SCAN

PINPOINT SHARED INFO between DATA SOURCES

MULTIMODAL REPRESENTATION LEARNING CAN GIVE A UNIFIED VIEW of A PATIENTS' HEALTH

## USING COHORT DATA to EXPLORE HEALTH & DISEASE

### JOINT EFFORT

PROVIDED ORGANISED, TOP-LEVEL METHODS

CLINICAL TRANSLATIONAL RESEARCH

GROWTH CHARTS for LUNG DEVELOPMENT ARE IMPORTANT!

7YO

COLLECTING DATA REPEATEDLY (OVER 50-60 YEARS) ALLOWED US TO BETTER UNDERSTAND COPD

LUNG HEALTH STARTS AT YOUTH!

WE NEED TO BUILD...

- FEEDBACK LOOPS
- OPEN NETWORKS
- SHARE RESULTS!

HOW to EVALUATE AI MODELS:

PROPERLY TEST the MODELS!

& FINE TUNE THEM

WE NEED to COLLABORATE

OUR ASPIRATIONS for AI in SCIENCE

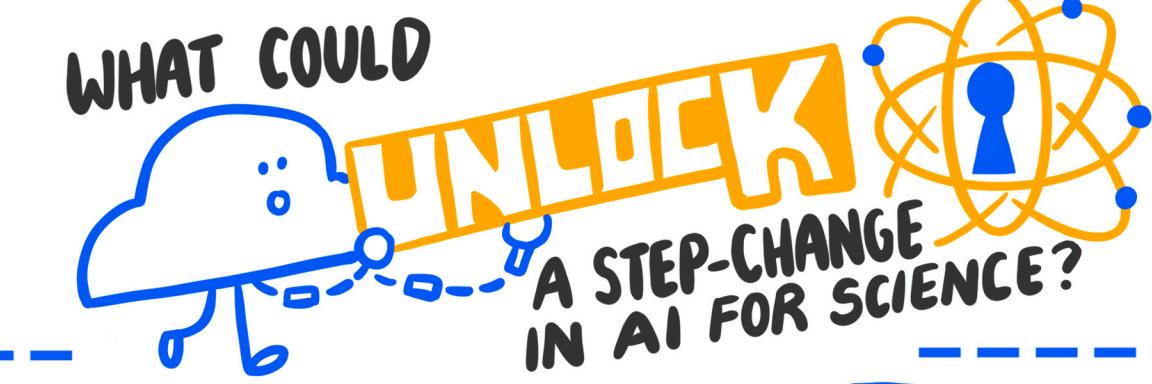
THINK ABOUT the LEGACY of the WORK WE LEAVE BEHIND!

JUSTIFY BENCHMARKS



# AI FOR SCIENCE SUMMIT

DAY 2: 26/11/24



## ASTRONOMY DATA

LARGE ARCHIVAL DATABASES, BUT SMALL LABELLED DATASETS

VARIABLE CLASS IMBALANCES

FOUNDATION MODELS: BEST "OWNED" by SAME COLLABORATIONS that OWN the DATA

REQUIRES BETTER VERIFICATION of OUTPUTS!

UNCERTAINTY GENERALISATION

ARE FOUNDATION MODELS REALLY the BEST SOLUTION for MULTI-MODAL DATA?

CAREFULLY CALIBRATE UNCERTAINTIES

BIASES IN MODELS

MULTI-MODAL MODELS

HIGHLY SPECIFIC USE CASES! ASTROCLIP ASTROM<sup>3</sup>

ASTRONOMY DATA ISSUES:

## AI for IMAGING

FROM DIFFERENTIAL EQUATIONS TO DEEP LEARNING for IMAGES

### EXCITING APPLICATIONS!

- REMOTE SENSING
- BIOMEDICAL: SPATIO-TEMPORAL MRI
- TRAFFIC MANAGEMENT
- VIRTUAL ART RESTORATION
- MODELLING PROTEIN DYNAMICS
- DIAGNOSIS/PROGNOSIS

DEEP LEARNING REVOLUTION CALLS for NEW APPROACHES & ASSOCIATED MATHEMATICS

MATHEMATICAL ROBUSTNESS

STRUCTURAL PROPERTIES

BIAIS

UNEXPLAINABILITY

UNPREDICTABLE behaviour

### LIMITATIONS & DANGERS of DEEP LEARNING

## improved REPEATABILITY

## DIVERSITY

WE NEED CONTINUITY

HOW DO WE EVALUATE the OUTPUTS?

CREATE A framework THAT HELPS!

## CHANGE the WAY WE WORK TOGETHER!

SHARE DA TA

WHAT KIND of SKILLS DO SCIENTISTS NEED?

## WE NEED to CREATE TOOLS that WORK!

WHAT COULD UNLOCK A STEP-CHANGE IN AI FOR SCIENCE?

BUILDING COMMUNITY & INSTITUTIONAL CAPABILITY

MORE SUPPORT for RSEs IN ACADEMIA