

I-X AI
 THEMED CAMPUS @ UNITE CITY
 BBC
 38 FELLOWS IN PLACE, ALREADY!
 YOU'RE HIRED!

Nick Jones
 IMPERIAL COLLEGE LONDON

What do the SCHMIDT FELLOWS Tell us about AI FOR SCIENCE?

BEN LAMBERT
 UNIVERSITY OF OXFORD

OUR MISSION
 WORLDWIDE ACROSS 9 UNIVERSITIES
 160 POST-DOC FELLOWS
 YEAR 1
 EVERY YEAR!

CROSS FERTILISE TO ALLOW STEM & AI TO CONNECT

NEIL LAWRENCE
 UNIVERSITY OF CAMBRIDGE

WE CAN'T MAP ALL PROTEINS ...
OUR GOAL
 Provide Capabilities

RESEARCH
 • Decipher ancient texts
 • design

Aha!
 HYPOTHESIS GENERATION

EXPERIMENT & DATA ANALYSIS

PEOPLE ARE LOOKING AT...

THEMES

- PDES, EMULATION & SIMULATION BASED INFERENCE
- MOLECULAR / MATERIAL DESIGN + DISCOVERY
- PURE MATHS + ML

PROGRESS

- 10 FELLOWS UNDERWAY...
- 15 NEW FELLOWS BEGINNING

OUR BRIDGING MODEL

ANYONE CAN JOIN! AT ANY STAGE!

COMMUNITY ENGAGEMENT
 50 RESEARCHERS!
 30 DEPTS!

BUT LESS REPRESENTATION ON

CAUSAL INFERENCE
 GRAPH NEURAL NETWORKS
 ROBOTICS
 GENOMICS

I'M WITH THAT THIS MADE ME DO IT

So many LANGUAGES

AI + SCIENCE MENTORS

WRITING TRAINING

SCHMIDT SOFTWARE REPOSITORY

NEW COHORT STARTS MAY 2024

300+ Participants
 80+ on data Pipelines

Tailored TRAINING

CHAIR: JESSICA MONTGOMERY
 UNIVERSITY OF CAMBRIDGE



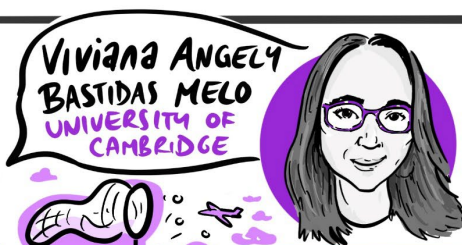
AI FOR SCIENCE

INSIGHTS FROM THE UK SCHMIDT FUTURES FUNDED CENTRES





ALEXANDRA BRINTRUP
UNIVERSITY OF CAMBRIDGE



VIVIANA ANGELY BASTIDAS MELO
UNIVERSITY OF CAMBRIDGE



SCOTT HOSKING
BRITISH ANTARCTIC SURVEY



JENNIFER SCHOOLING
UNIVERSITY OF CAMBRIDGE

DATA SHARING IS A CHALLENGE IN SUPPLY CHAINS

Dealing with Sensitive Information
CLASSIFIED



INCENTIVIZE SHARING

WE NEED TO APPEAL TO INDUSTRY & ACADEMIA

IS PUBLISHING

BROKEN?

OXFORD. IMPERIAL CAMBRIDGE. IF WE CAN'T CHANGE IT, WHO WILL?

We're incentivised to IMAGINE & ANSWER questions NOONE'S asking



CHAIR: NEIL LAWRENCE



COLLECTING DATA IN CITIES IS A CHALLENGE!



PRIVACY TRUST

eg. failure of SIDEWALK PROJECT

WE MUST UNDERSTAND COMMUNITIES BETTER

COLLABORATE ACROSS DISCIPLINES



Solved it!



UHUH.



GRAND CHALLENGES IN AI FOR SCIENCE

We have fewer sensors in ANTARCTICA than a LONDON STREET



WEATHER FORECASTS

YOU KNOW IT'S GONNA BLOW SO MODEL THE EVACUATION

GET A SIMULATOR IN THE LOOP to better resemble the PHYSICS

AI Needs more sophisticated understanding - eg of TUNNELS BELOW

It is vital to THINK ON WHERE FOCUS OUR ENERGIES

FALLING VIADUCT



Bottleneck

AI CAN SPOT IT BUT NEEDS A HUMAN TO UNDERSTAND IT

Typically you need to EXPLAIN a SYSTEM



WHAT MAKES A WAVE BREAK? HOW MACHINE LEARNING CAN SHED LIGHT ON THE UNDERLYING PHYSICS OF BREAKING WAVES



TIM TANG
UNIVERSITY OF OXFORD



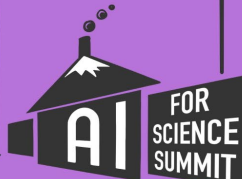
- OUR EQUATION SUGGESTS NEW CHARACTERISTIC OF BREAKING WAVES AND HINTS AT MUCH CHEAPER WAYS TO COMPUTATIONALLY SIMULATE BREAKING WAVES (W.I.P!)

RESULTS ARE VERY FAST!

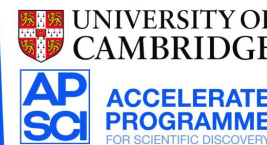
2 MINUTES ON A DESKTOP VS. 3259 CORE HOURS ON A SUPER COMPUTER

When wave amplitude reaches CRITICAL POINT that the CREST self-dissassembles

FIND OUT MORE



EMPLOYING AI TO IDENTIFY THE COMPLEX INTERACTIONS OF ENVIRONMENTAL STRESSORS ON POLLINATOR HEALTH



RACHEL PARKINSON
UNIVERSITY OF OXFORD



- SOUND IS A TYPICALLY OVERLOOKED ASPECT OF INSECT BEHAVIOUR
- I'VE CONSTRUCTED A RECORDING ARENA FOR HIGH-THROUGHPUT DATA ACQUISITION FROM INSECTS

I'M DEVELOPING A MULTI-MODAL ML ALGORITHM THAT AUTOMATICALLY TRACKS BEHAVIOUR. This system QUANTIFIES the effects of ENVIRONMENTAL STRESSORS!

Tracking behaviour through SOUND AND VIDEO!



FIND OUT MORE



MATHEMATICAL CONJECTURE GENERATION & MACHINE INTELLIGENCE



CHALLENGER MISHRA

UNIVERSITY OF CAMBRIDGE

- GOOD CONJECTURES HAVE HISTORICALLY INSPIRED NEW MATHEMATICS AND SHAPED PROGRESS IN THEORETICAL PHYSICS

Machine learning is TAILOR-MADE to solve problems in PATTERN RECOGNITION

A NEW FRAMEWORK

FOR A PRINCIPLED STUDY OF THIS SPACE, WITH DOMAIN KNOWLEDGE AND MACHINE LEARNING

GENERATES = NON TRIVIAL = CONJECTURES

IN GROUP THEORY & NUMBER THEORY

HILBERT'S 23 PROBLEMS



Find out more →



AI-ENHANCED SYNTHESIS TO SAVE BIODIVERSITY



ALEC CHRISTIE

UNIVERSITY OF CAMBRIDGE

- LARGE-SCALE SYNTHESIS METHODS ARE TOO MANUAL & TOO SLOW
- AI CAN VASTLY SPEED UP SYNTHESIS PIPELINE TO ACCELERATE THE COMMUNICATION OF EVIDENCE TO KEY DECISION-MAKERS



PROJECT 1

INCLUDING DECISION SUPPORT

PROJECT 2

AUTOMATE EVIDENCE SYNTHESIS PIPELINE

DETECT INVASIVE SPECIES

AND PESTS

USING SOCIAL MEDIA + NEWS SITES

Find out more →



CUSTOMISING 3D CELL SEGMENTATION TO STUDY PREIMPLANTATION MOUSE EMBRYOS

UNIVERSITY OF
CAMBRIDGE

AP
SCI ACCELERATE
PROGRAMME
FOR SCIENTIFIC DISCOVERY

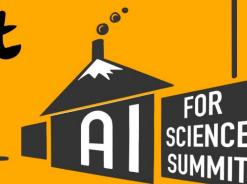
ANITA
KARSA
UNIVERSITY OF
CAMBRIDGE

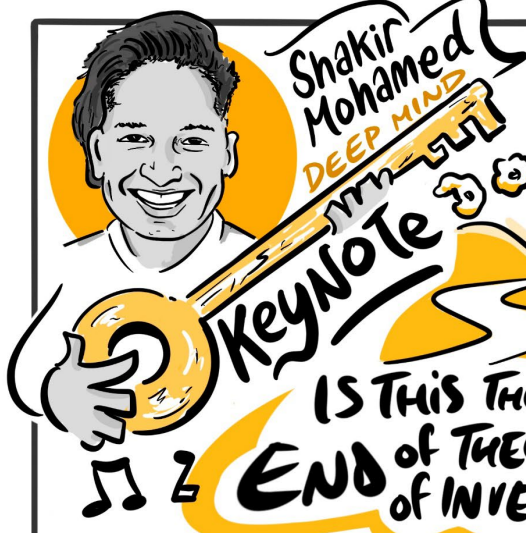
- BIOLOGISTS GET INSIGHTS ON FERTILITY BY STUDYING THE PRE-IMPLANTATION DEVELOPMENT OF MOUSE EMBRYOS
- 3D CELL SEGMENTATION IS KEY TO THIS IMAGE ANALYSIS BUT MANUAL SEGMENTATION TAKES SEVERAL DAYS

We trained
STARDIST 3D
on mouse embryo data
to get accurate 3D cell
segmentation in UNDER

20 MINUTES!

Find out
more





1 Pace + Progress IN SCIENCE

IS THIS THE END OF THEORY? END OF INVENTION?

Bias • CALIBRATION • UNFAIRNESS
THE DATA CAN'T SPEAK FOR ITSELF ... YET.

CONCEPTUAL FRAMING OF EVALUATION

Mixed Methods of Evaluation
TECHNICAL AUTOMATIC QUANTITATIVE
QUALITATIVE PEOPLE-FOCUSED

2 Science Assistants + Knowledge Production

STILL a CREATIVE PROCESS
HOW MAKE TOOLS MORE PEOPLE-CENTRED?
Social Context
SCIENCE RESEARCH
EMPIRICAL LIKELIHOOD
A classic idea that is just as relevant today

4 Responsibilities of the Pioneer

FORECAST ACCURACY FORECAST EQUITY
EL NINO LEADS TO LANDOFFS
FORECASTS CAN HARM NOT HELP COMMUNITIES
FORECASTS ARE LESS 25% ACCURATE FOR LOW-INCOME COUNTRIES
PIONEERS WE ARE THE PEOPLE WHO'LL DEFINE THE FRONTIER!

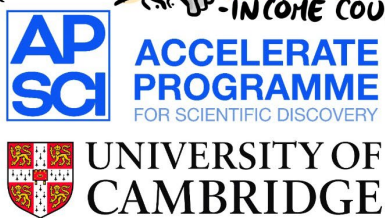
PERFORMANCE SCORECARD
GRAPHCAST is better on 90% of targets
IN 60 SECONDS!
Weather Forecasting
The MAGIC INGREDIENT IS ECMWF FORECAST DATA
EXTREME HEAT

3 Scientific Simulation

EARTH SYSTEM MODELS is a Great area to DIVE INTO!

GENERATIVE SCIENCE

ROLES FOR GENERATIVE AI IN SCIENTIFIC DISCOVERY



1 LAW

THE TIME GAP (SLOW vs FAST)

2 How Regulate an ENDLESS PROTOTYPE?

3 How Assess UNKNOWN RISK when HUMANS in the Frame?

GOOD REGULATION IS VITAL TO TRUST

DISCUSSION TOOLS

Protect THE ARTIST

data SOURCES can be SO DIVERSE

GIOVANNI BANDI UNIVERSITY OF CAMBRIDGE

IT'S FOR RESEARCH? SURE!

2021

2023

LLM ERA

LEARN INTO THE SPICE

WE WERE THE BAD GUYS ONCE...!

OPEN VS NOT OPEN

SOCIETY EXPECTS INNOVATION

HOW DO WE DECENTRE POWER?

SPICY CHIPS

Go and Meet Social Scientists

...BUT DON'T GO CRAZY!

SHAKIR MOHAMED DEEP MIND

MAYA INDIRA GANESH UNIVERSITY OF CAMBRIDGE

KEY ROLE FOR INSTITUTIONS

PRINCIPLES ...and the FUZZY STUFF

NARRATIVES

HOW YOU DO IT?

Check list

TRUST

ENGLISH LANG. SKILLS

FREE GPT

PAID GPT

OPPORTUNITIES AROUND ACCESSIBILITY

What's our INFRASTRUCTURE around HARM?

PANEL DISCUSSION



REFLECTIONS ON LLMs & AI FOR SCIENCE



EMPLOYING AI TO IDENTIFY THE COMPLEX INTERACTIONS OF ENVIRONMENTAL STRESSORS ON POLLINATOR HEALTH

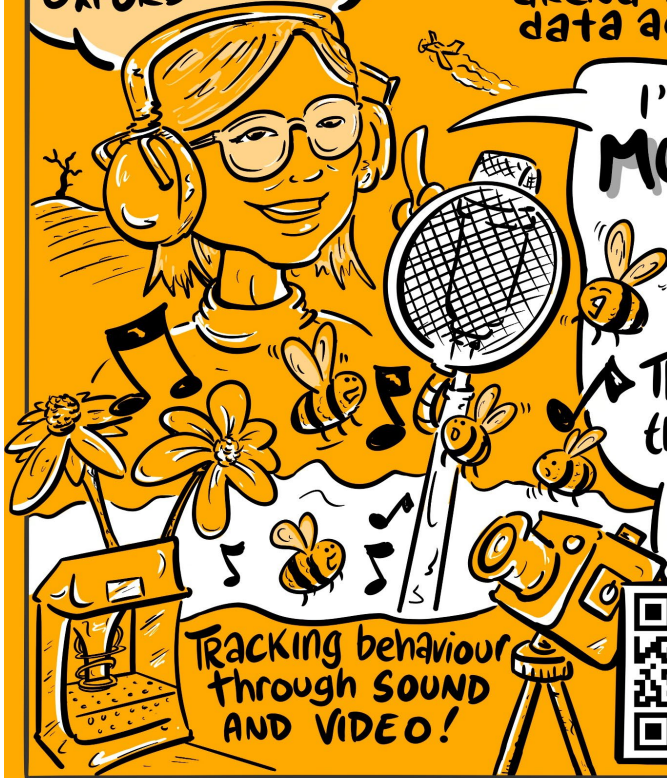


RACHEL PARKINSON
UNIVERSITY OF OXFORD

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Find out more



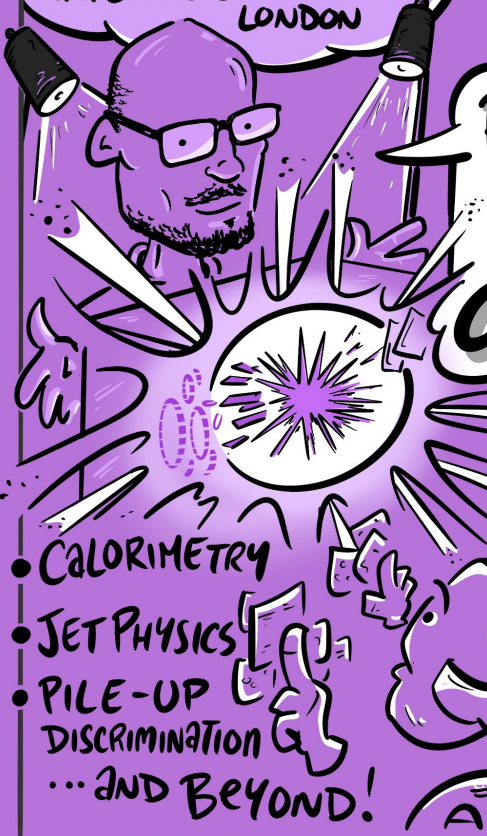
HYPERTRACK: NEURAL COMBINATORICS FOR HIGH-ENERGY PHYSICS



MIKAEL MIESKOLAINEN
IMPERIAL COLLEGE LONDON

- A NEW DEEP-LEARNING-DRIVEN CLUSTERING ALGORITHM THAT UTILISES A SPACE-TIME NON-LOCAL TRAINABLE GRAPH CONSTRUCTOR, A GRAPH NEURAL NETWORK AND A SET TRANSFORMER

PARTICLE TRACKING SIMULATIONS SHOWCASE THE EFFECTIVENESS OF THIS CUTTING EDGE APPROACH

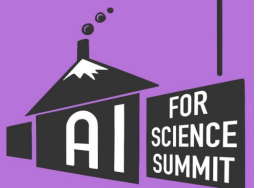


- CALORIMETRY
- JET PHYSICS
- PILE-UP DISCRIMINATION
- ...AND BEYOND!

Next Frontier

Develop model to capture degrees of freedom, able to describe transitions from elementary particles through to galaxy clusters

Find out more



A MULTISCALE GENERATIVE MODEL UNVEILS DISORDER IN DOMAIN BOUNDARIES

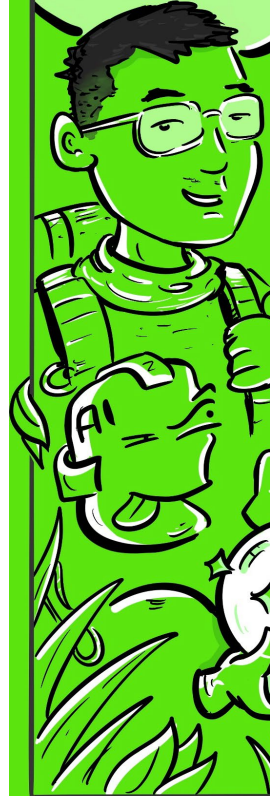


JIADONG DAN

NATIONAL UNIVERSITY OF SINGAPORE

A CRITICAL CHALLENGE IN ATOMIC RESOLUTION MICROSCOPY IS IDENTIFYING STRUCTURAL MOTIFS IN SYNTHESISED MATERIALS

We introduce a novel **HYBRID GENERATIVE MODEL** to **PREDICT UNSEEN DOMAIN BOUNDARIES**



ML MODELS CAN DECIPHER DISORDER IN COMPLEX MATERIALS, ENABLING **ADVANCES IN FUTURE FUNCTIONAL MATERIALS DESIGN**

Find out more →



IMAGE-BASED AI DIAGNOSIS PLATFORM FOR EARLY DROUGHT STRESS DETECTION IN PLANT LEAVES

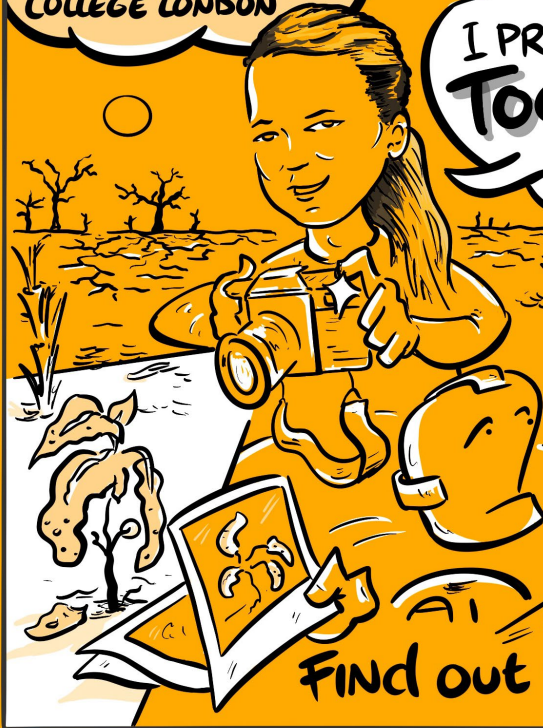


ALICE MALIVERT

IMPERIAL COLLEGE LONDON

- DROUGHT STRESS IS CAUSE OF **OVER 34%** OF CROP LOSS IN DEVELOPING AND LEAST DEVELOPED COUNTRIES
- WE MUST DETECT THE FIRST SIGNS QUICKLY AND COST-EFFICIENTLY

I PROPOSE AN **AI-ASSISTED TOOL** TO DETECT EARLY SIGNS OF DROUGHT STRESS IN PLANT LEAF PICTURES



ULTIMATE RESULT IS OPEN ONLINE PLATFORM TO DIAGNOSE DROUGHT STRESS IN PLANT LIFE PICTURES FOR **RESEARCHERS AND FARMERS ALIKE!**

Find out more →

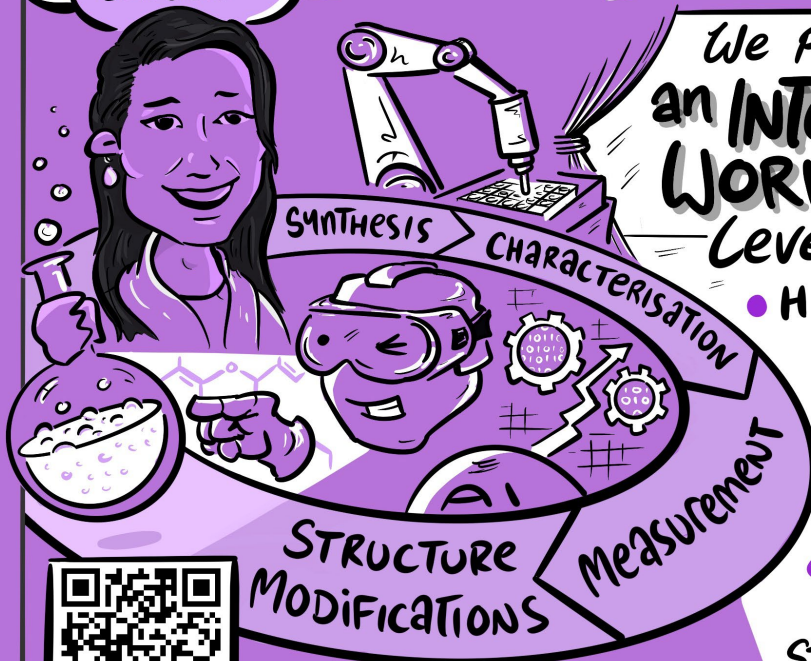


TOWARDS A GENERALISED PLATFORM FOR AI-DRIVEN ACCELERATION OF CLOSED-LOOP CHEMICAL DISCOVERY



AUSTIN MROZ
IMPERIAL COLLEGE LONDON

- WE NEED NOVEL CHEMICAL SYSTEMS GIVEN THE CLIMATE EMERGENCY, RESOURCE SCARCITY & ENERGY CONSUMPTION NEEDS
- TRADITIONAL 'TRIAL-AND-ERROR' DISCOVERY TAKES UP TO 20 YEARS PER NEW MATERIAL!



We present...
an INTEGRATED WORKFLOW,
Leveraging...

- HIGH-THROUGHPUT **AUTOMATED** EXPERIMENTS
- **ABSTRACT** COMPUTATIONAL MODELS
- **DATA-DRIVEN** OPTIMIZATION STRATEGIES

Find out more

scribeyesense.com





NICK JONES
IMPERIAL COLLEGE LONDON


THERE'S AN OPPORTUNITY FOR **CONVERGENCE** BETWEEN **MATHEMATICS** AND **SCIENCES**

INTERPRETABILITY = **Black Box** TO **TEXT / BOOK**

THE AI REVOLUTION HASN'T ARRIVED YET...



CHAIRER BY **CARL HENRIK EK**



MARK GIROLAMI
UNIVERSITY OF CAMBRIDGE • ALAN TURING INSTITUTE

(eg **NEUROSCIENCE** / **CARBOHYDRATE**)

AI IS A **SCIENCE** IN ITS OWN RIGHT!!

THE IMMENSE DATA POWER OF NEW TECH LEAVES REST IN SHADE RIGHT NOW... but potentials **HUGE**

Science is **HARD-NOSED** time whittles out the weak

BRIDGES! PLANES! AI NEXT?

NO ONE SAYS 'AI' THESE DAYS!

Calculus
Deep Learning

2033

PANEL DISCUSSION



JOHN ASTON
UNIVERSITY OF CAMBRIDGE

You must work on things like **GROUP THEORY** to understand AI

AI Models

Share + Extend OUT OUR SILOS.

TRY IT! TEST IT... BUT then Go Back and EXPLORE the **WHY** and get the **CREDIT**



ZOE KOURTZI
UNIVERSITY OF CAMBRIDGE

AI has totally **REVOLUTIONISED** how we understand **COMPLEX SYSTEMS** like the **HUMAN BRAIN**

ITS A **BRIDGE** TO NEW IDEAS

A LOT OF **GREAT TOOLS** stay on **SHELF** without a **GOOD** well-understood **NARRATIVE**

NEUROSCIENCE **NEEDS AI**

Beyond the dish

THE SCIENCE OF AI FOR SCIENCE




ALESSANDRO TREVISAN
UNIVERSITY OF CAMBRIDGE

Interdisciplinarity

70 YRS
NO CLARITY ON COPYRIGHT LAW FOR LLMs

CHALLENGE
ACCESSING GPU POWER

LLMs STRUGGLE TO IDENTIFY GOOD STORIES



CHAIR: CATHERINE BRESLIN
KINGFISHER LABS
UNIVERSITY OF CAMBRIDGE




We ALL HAVE a USE for LLMs

Reading Writing

A CHALLENGE
INSUFFICIENT DETAIL TO BUILD ON RESEARCH.

CAN LLMs help with this?

BENCHMARKS?
MOVE FROM multi-choice TO open ended narrative



MARION SHORT
UNIVERSITY OF CAMBRIDGE

AI IS USEFUL TERM IN CHEMISTRY



A human eye skill needed so you're back to SQUARE ONE!

OPTIMISE PROMPT? VS FINE TUNE MODEL

PROMPTS LET IN BIAS



PETRE BREAZU
UNIVERSITY OF CAMBRIDGE

Open-ness and Clarity

Collaboration



Journal
Aless
IKEA
You Need a mix of QUAL + QUANT

PUBLISHING LAGS BEHIND SPEED OF LLM DEVELOPMENT



SOON ENOUGH YOU CAN SPOT GPT'S STYLE

A CHALLENGE FINDING NETWORKS

STUDY GROUPS HELP

UNWORKSHOP 1

LLMs & AI FOR SCIENCE





CATHERINE BRESLIN
KINGFISHER LABS
UNIVERSITY OF CAMBRIDGE



EMILIO MONTI
AMAZON



SAMIA MOHINTA
UNIVERSITY OF CAMBRIDGE



RYAN DANIELS
UNIVERSITY OF CAMBRIDGE

AP SCI ACCELERATE PROGRAMME FOR SCIENTIFIC DISCOVERY



UNWORKSHOP 2

BEST PRACTISES IN SOFTWARE ENGINEERING





State of the Art

Challenges "PDFs in 2023?"

Career Advice



NEIL LAWRENCE
UNIVERSITY OF CAMBRIDGE

HIGH LIGHT

FLASH TALKS

BREADTH DEPTH

THE EXCITEMENT AROUND AI IS A CHANCE TO ADDRESS THE ISSUES AROUND INTERDISCIPLINARY

Even the Greeks had SCROLLING!



ONLY APPLY TACTICS TO SOMETHING YOU CARE ABOUT!
DON'T JUST DO IT FOR THE MONEY



BEN LAMBERT
UNIVERSITY OF OXFORD

BE OPEN PIONEERS
THE RESPONSIBILITY TO DOCUMENT

RULES
#1. DON'T FOOL YOURSELF

The solution is CONVERSING as a DIVERSE COMMUNITY

YOU MUST BE INTO THE TOPIC, NOT JUST FILLING A HOLE FOR OTHERS

PERSONAL MOTIVATION!
FOR ME, THAT MEANT 10 YEARS OF STATISTICS VIDEOS!
WALK OWN PATH



NICK JONES
IMPERIAL COLLEGE LONDON

NUMERICAL ANALYSIS
THE FUSION WITH

'REPRODUCIBILITY DIGEST'
A NEW TYPE OF PAPER
COMBINING WORK FROM DISTINCT TEAMS REPRODUCING RESULTS

FORMULATE a RESEARCH VISION



DIVERSITY THROUGH MATERIALS

WHY WOULD I STAY?
CULTURE TRADITION

PASSIVITY IS AN INSUFFICIENT RESPONSE

ACKNOWLEDGE IN YOUR ROLE AND WORK

TIME WILL CHANGE THINGS

FIRESIDE CHAT

INTERVIEWED BY:



CHALLENGER MISHRA • SARAH MORGAN
UNIVERSITY OF CAMBRIDGE

