An inspirational forward-looking generative & well-seasoned perspective on the denoised adjacent possible

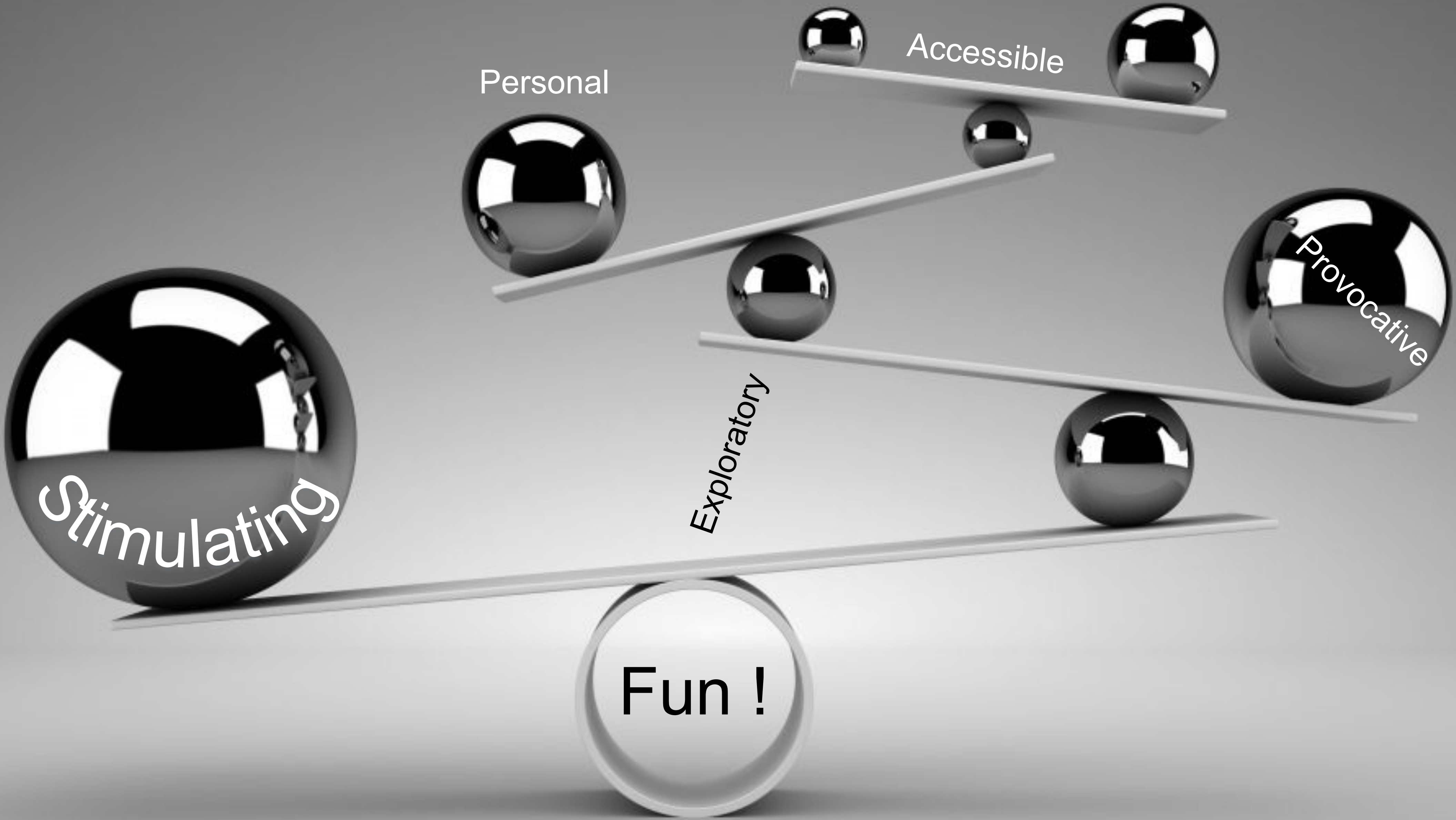
Tobias Golling

UNIVERSITÉ
DE GENÈVE

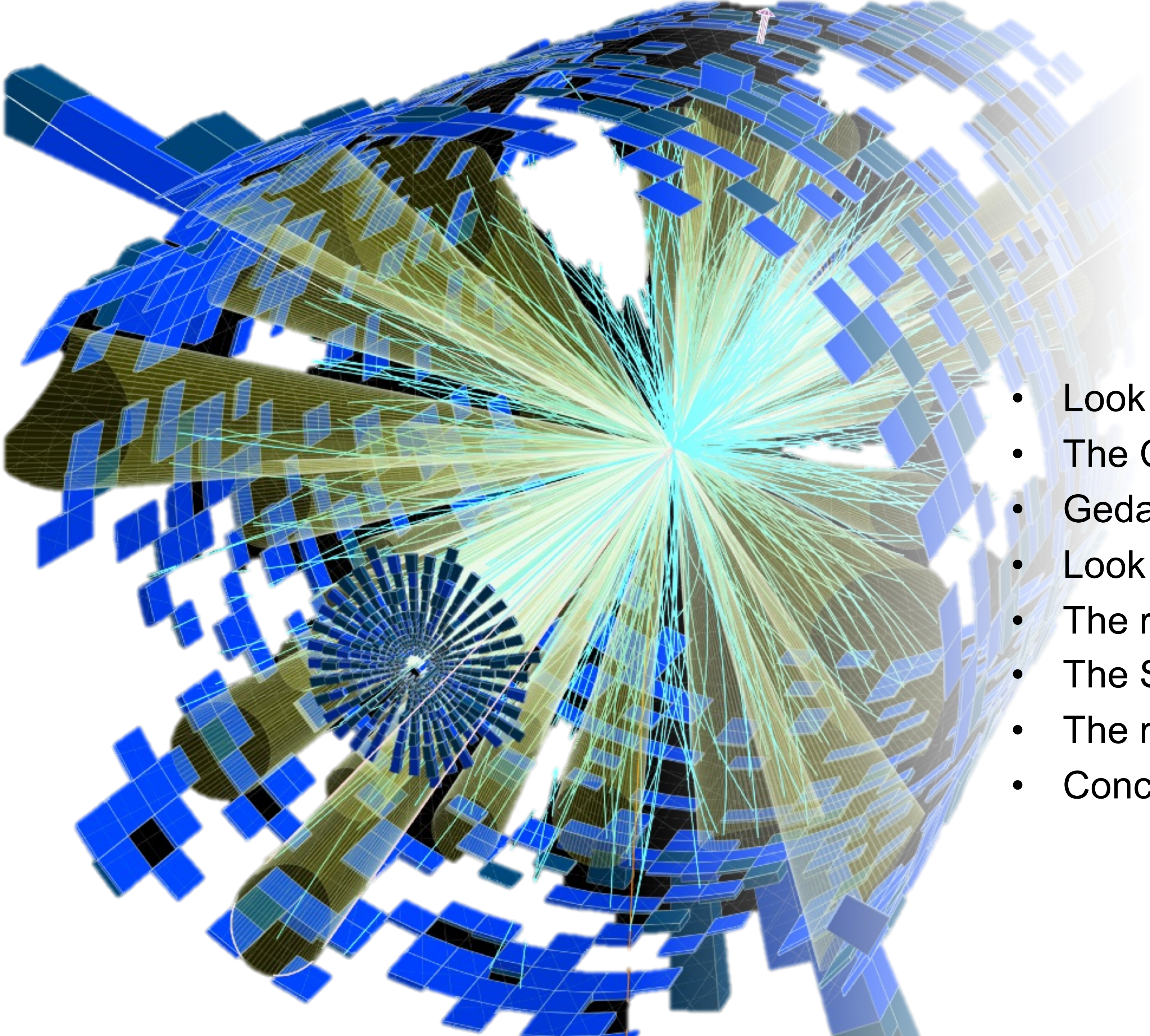
Focus on Big Picture

Thanks to organizers who gave me a *blank check*

- ML…LHC…unique perspective


Accessible
Personal
Provocative
Exploratory
Stimulating
Fun !


Snapshot
Biased
ATLAS-centric
Too long, but incomplete
a good steal
is half
the battle



Outline

- Look back & ahead
- The Challenges
- Gedankenexperimente
- Look to the Data
- The role of Theory
- The Strategy
- The role of Experiment
- Concluding remarks

Pat on the back

ML@HEP = widespread impact

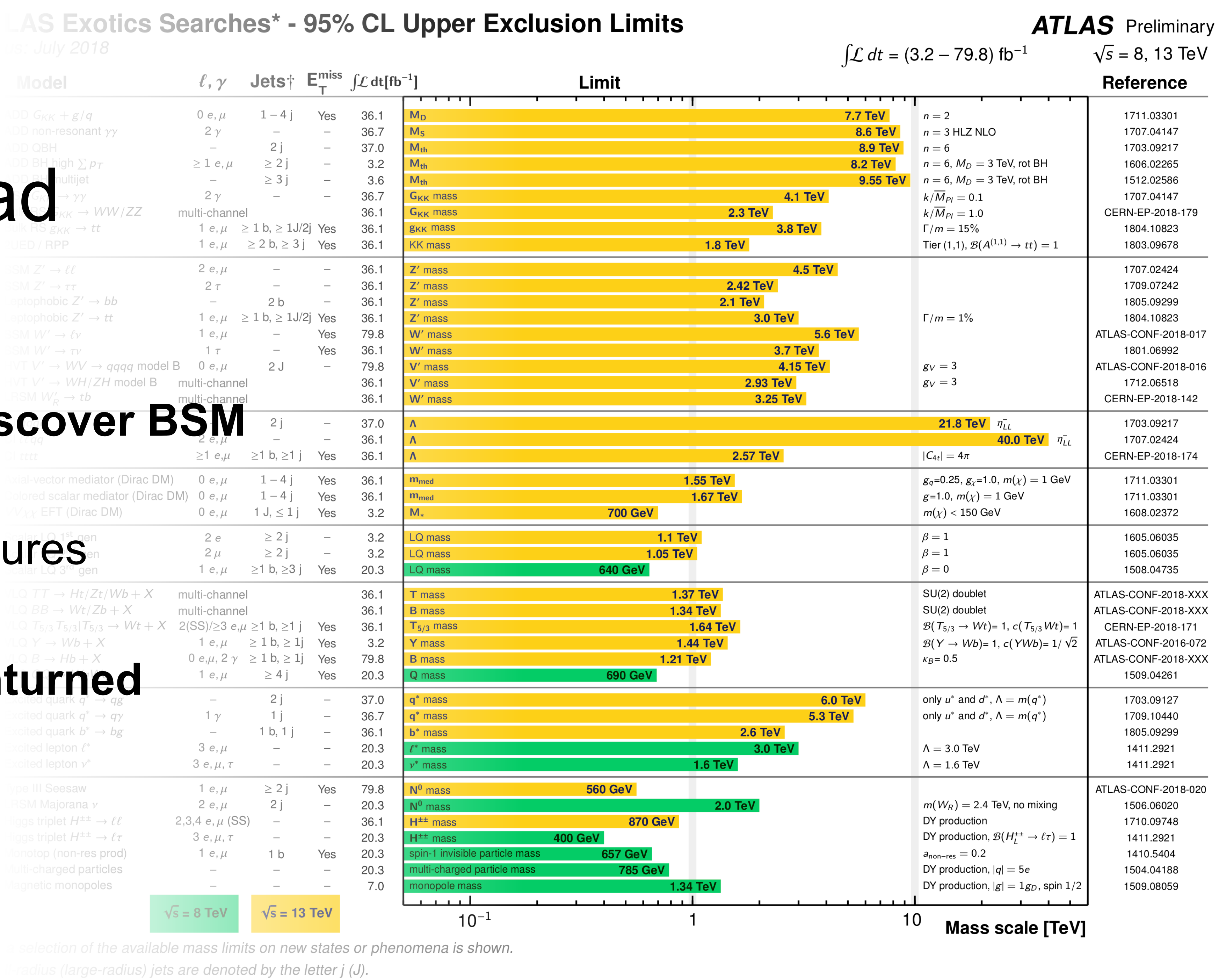
Contributions well beyond our field

A look ahead

Main purpose of LHC: **discover BSM**

Hypothesis: *subtle* signatures

Obligation: no stone unturned



New search portfolio is **diverse** & powered by **ML**

Concrete challenges

Computing (simulation, on-the-edge,…)

Modeling (pileup, reco,…)

Human resources*

ATLAS + CMS = O(1000) search papers
~2 years per analysis
Average of 4 people
8000 person years

[*inspired by talk by Shikma Bressler, Hammers & Nails ’22]

Let’s unpack the challenges

Core Challenge: vast signature space **un**explored

	e	μ	τ	q/g	b	t	γ	Z/W	H	BSM $\to$ $SM_1 \times SM_1$				BSM $\to$ $SM_1 \times SM_2$				BSM $\to$ complex			
										q/g	γ/π^0's	b	$\cdots$	tZ/H	bH		$\cdots$	$\tau qq'$	eqq'	$\mu qq'$	$\cdots$
e	[37, 38]	[39, 40]	[39]	∅	∅	∅	[41]	[42]	∅	∅	∅	∅		∅	∅	∅		∅	[43, 44]	∅	
μ		[37, 38]	[39]	∅	∅	∅	[41]	[42]	∅	∅	∅	∅		∅	∅	∅		∅	∅	[43, 44]	
τ			[45, 46]	∅	[47]	∅	∅	∅	∅	∅	∅	∅		∅	∅	∅		[48, 49]	∅	∅	
q/g				[29, 30, 50, 51]	[52]	∅	[53, 54]	[55]	∅	∅	∅	∅		∅	∅	∅		∅	∅	∅	
b					[29, 52, 56]	[57]	[54]	[58]	[59]	∅	∅	∅		[60]	∅	∅		∅	∅	∅	
t						[61]	∅	[62]	[63]	∅	∅	∅		[64]	[60]	∅		∅	∅	∅	
γ							[65, 66]	[67–69]	[68, 70]	∅	∅	∅		∅	∅	∅		∅	∅	∅	
Z/W								[71]	[71]	∅	∅	∅		∅	∅	∅		∅	∅	∅	
H									[72, 73]	[74]	∅	∅		∅	∅	∅		∅	∅	∅	
BSM $\to$ $SM_1 \times SM_1$: q/g										∅	∅	∅		∅	∅	∅		∅	∅	∅	
BSM $\to$ $SM_1 \times SM_1$: γ/π^0's											[75]	∅		∅	∅	∅		∅	∅	∅	
BSM $\to$ $SM_1 \times SM_1$: b												[76, 77]		∅	∅	∅		∅	∅	∅	
$\vdots$																					
$\vdots$																					

Multi-body final states, unconventional signatures… ⚡

[1907.06659]

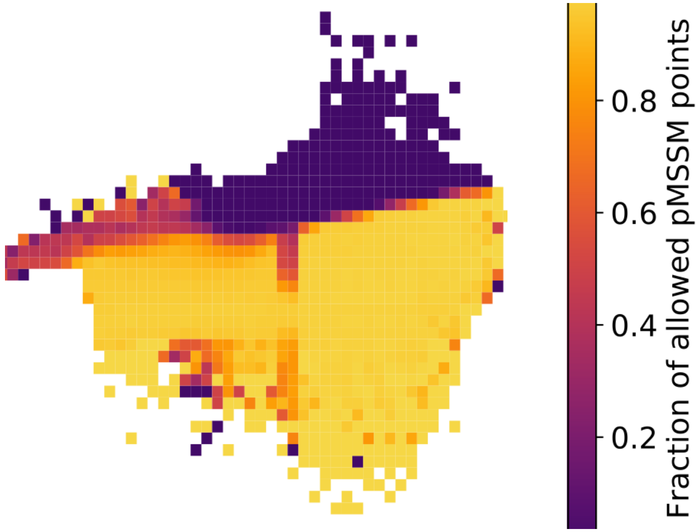
Two complementary approaches

Theory at face value

e.g. MSSM (105) → **pMSSM (19)**

Strong physics bias

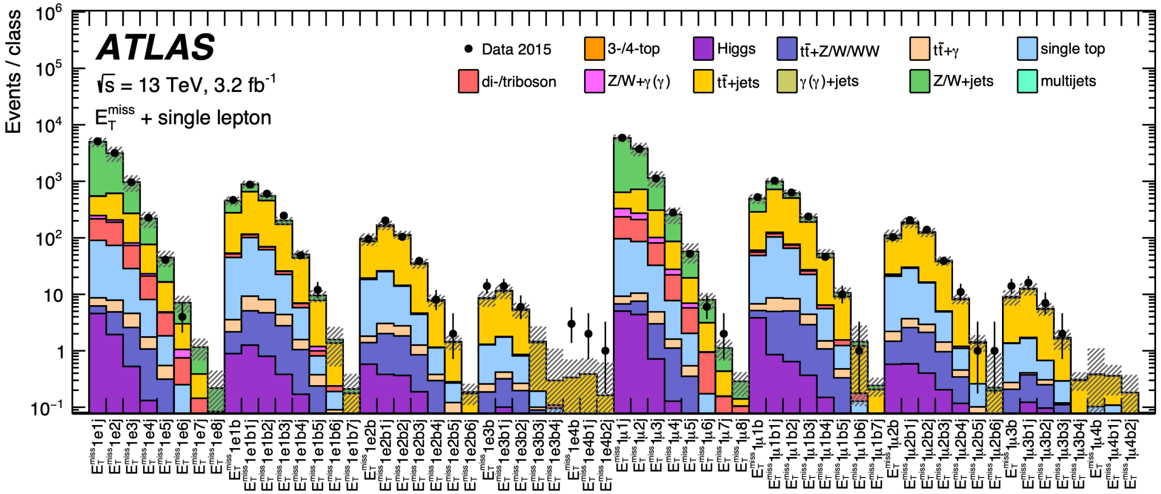
Smart sampling



[2207.05103]

Model-agnostic signature-based

e.g. [1807.07447]



10^5 signal region

Limitations

MC mismodeling

Only cut and count

Look elsewhere effect

Pros & Cons

Theory guided: forward modeling

Interpret ✅

Incomplete signatures space ⭕

[Courtesy of Hitoshi Murayama]

	e	μ	τ	q/g	b	t	γ	Z/W	H	BSM $\to$ SM$_1$ $\times$ SM$_1$				BSM $\to$ SM$_1$ $\times$ SM$_2$				BSM $\to$ complex			
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γ							[65, 66]	[67–69]	[68, 70]	∅	∅	∅		∅	∅	∅		∅	∅	∅	
Z/W								[71]	[71]	∅	∅	∅		∅	∅	∅		∅	∅	∅	
H									[72, 73]	[74]	∅	∅		∅	∅	∅		∅	∅	∅	
BSM $\to$ SM$_1$ $\times$ SM$_1$: q/g										∅	∅	∅		∅	∅	∅		∅	∅	∅	
γ/π^0's											[75]	∅		∅	∅	∅		∅	∅	∅	
b												[76, 77]		∅	∅	∅		∅	∅	∅	
$\vdots$																					
$\vdots$																					

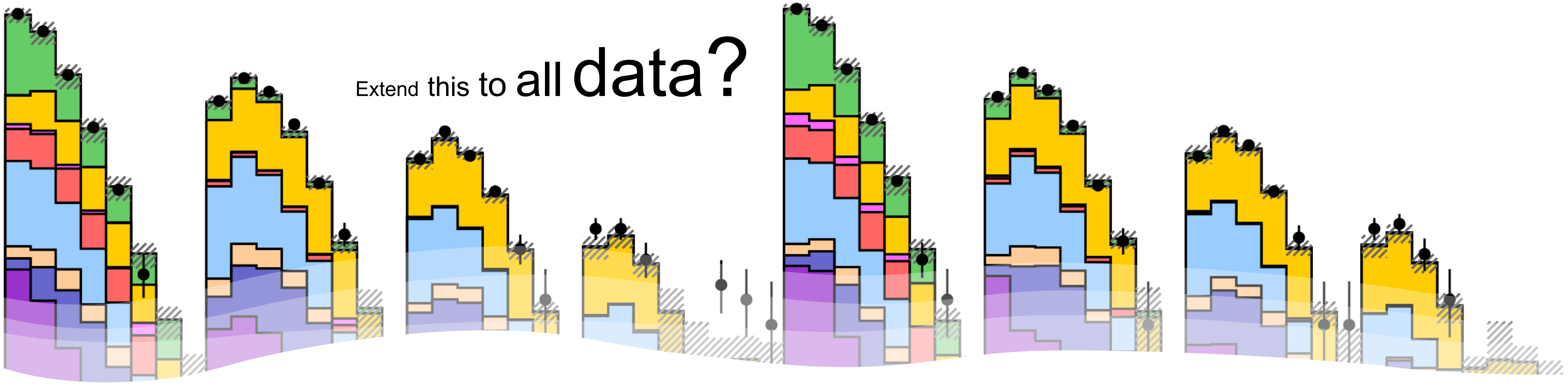
Model-agnostic:

Interpret ⭕

Scan *all* signature space → *data-driven* ✅

What if we had perfect modeling

Extend this to all data?



Data slicing?

Does this scale?

Look elsewhere

→ Data-driven

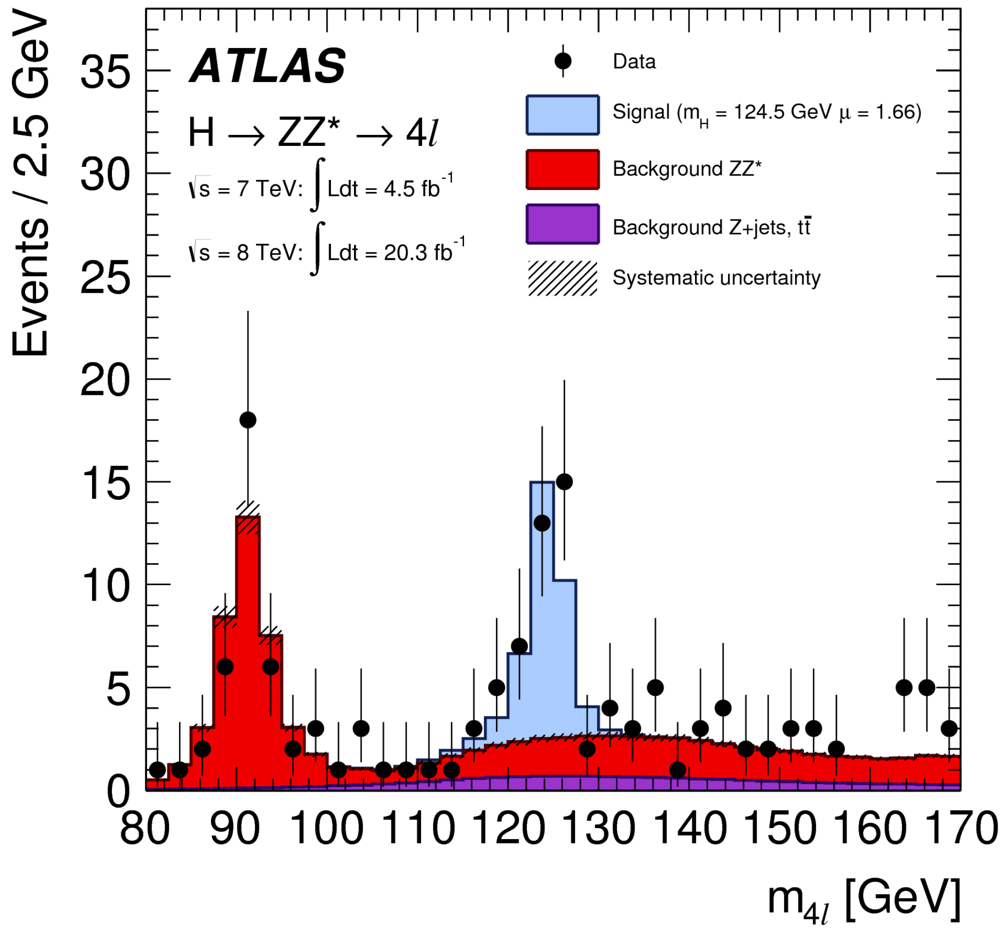
What if we had infinite compute & storage

The human factor

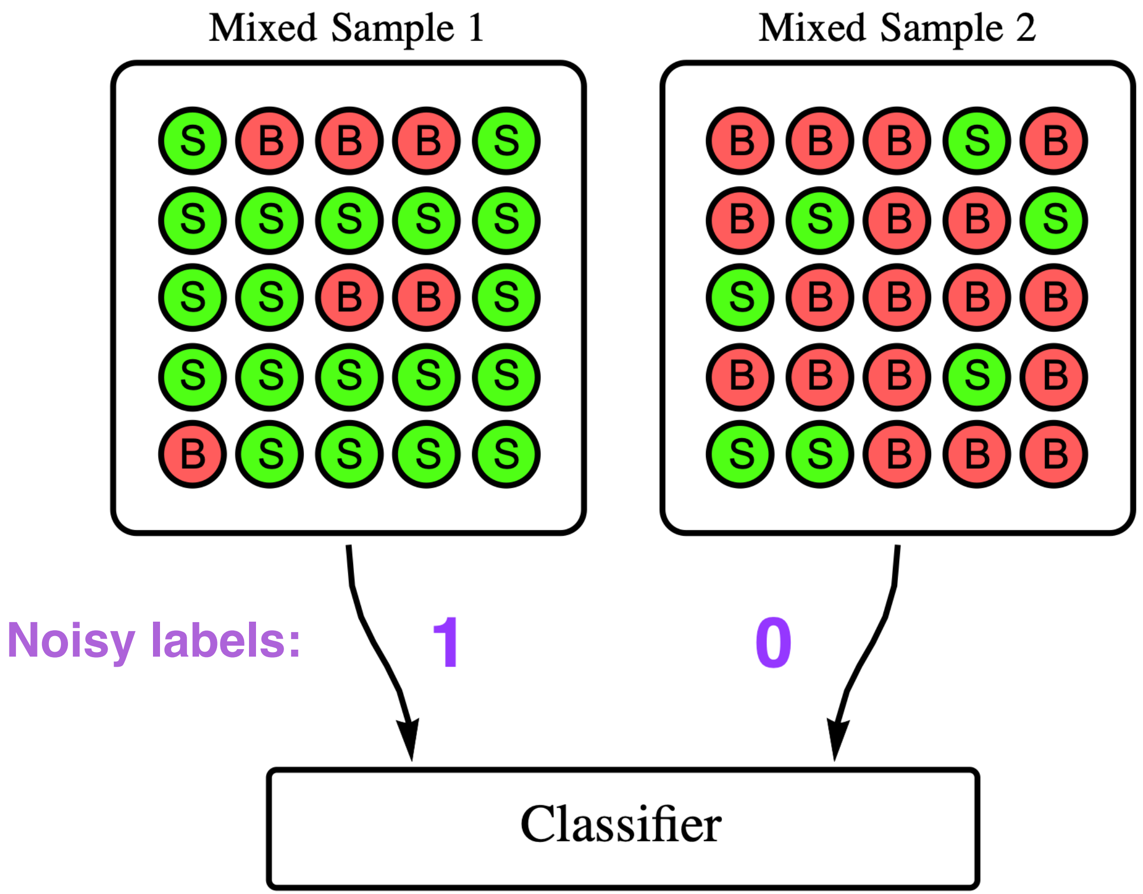
A word on *labels*

No notion of *event label*

Only *probability* to be S or BG



Classification without labeling (CWoLa)



[1702.00414, 1708.02949]

Feature space = prior

Bump hunt [1902.02634]

ATLAS analysis [2005.02983]

Beyond resonances

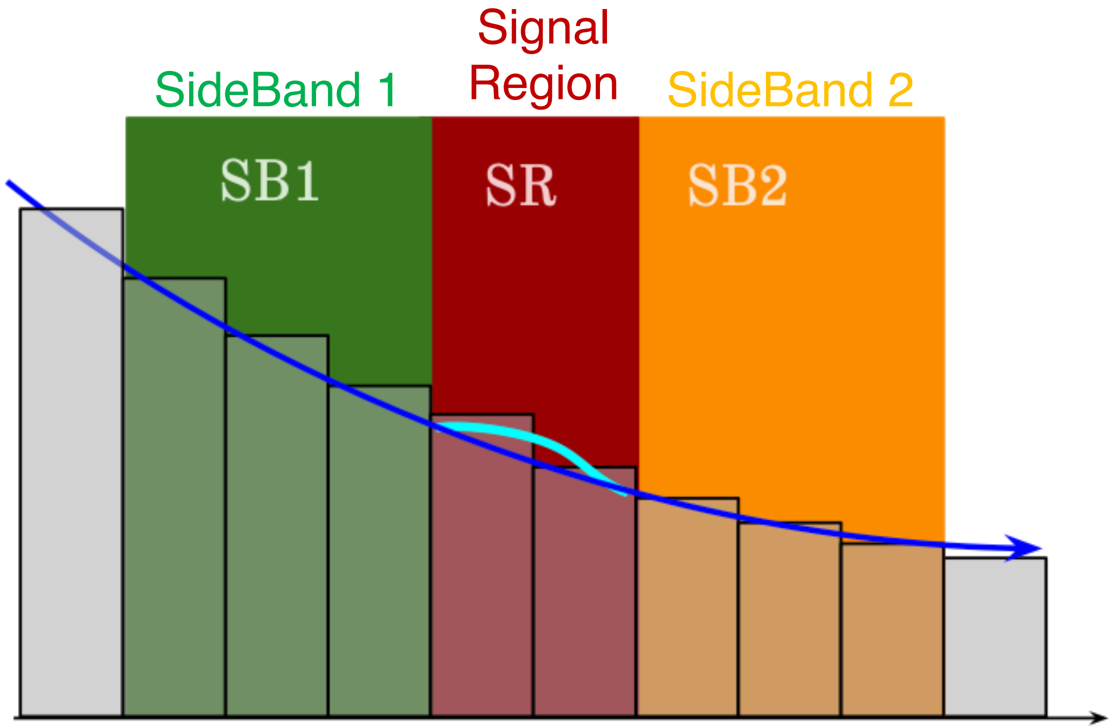
e.g. symmetries [2203.07529]

The CWoLa spirit: *all in data*

Main challenge: calibration

Background calibration in bump hunt

Interpolate BG *template* from SB's to SR



Calibration methods

Matrix method: no signal enhancement possible ⚡

Traditional interpolation: high feature space ⚡

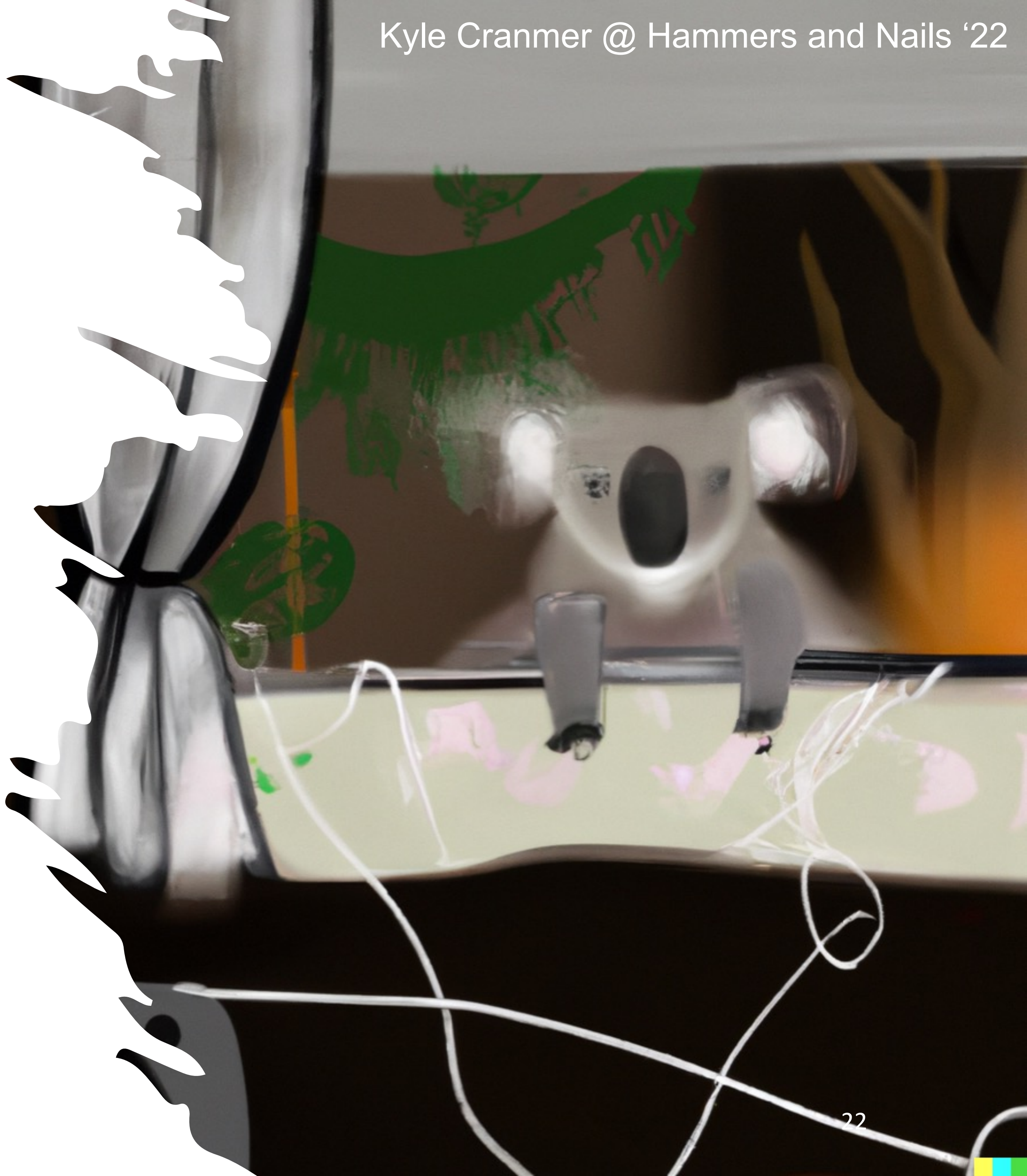
Density estimates: ANODE, CATHODE, LaCATHODE*

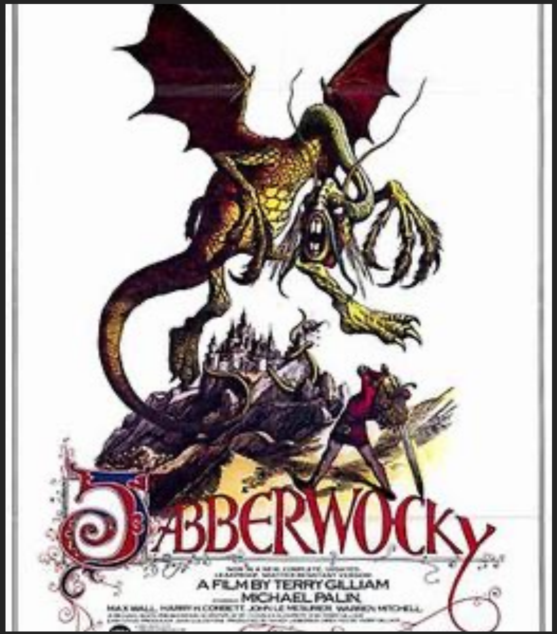
Transform BG template: CURTAINs & update*

Hybrid BG in MC morphed to data: SALAD & variation*

*talks by Manuel Sommerhalder, Johnny Raine, Radha Mastandrea

La
CWo-CUR-CATH-LAD





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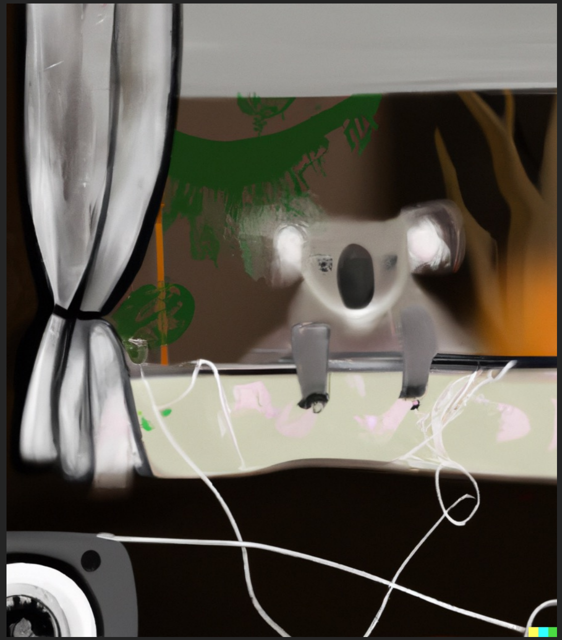


Mix & match

Room to optimize & extend

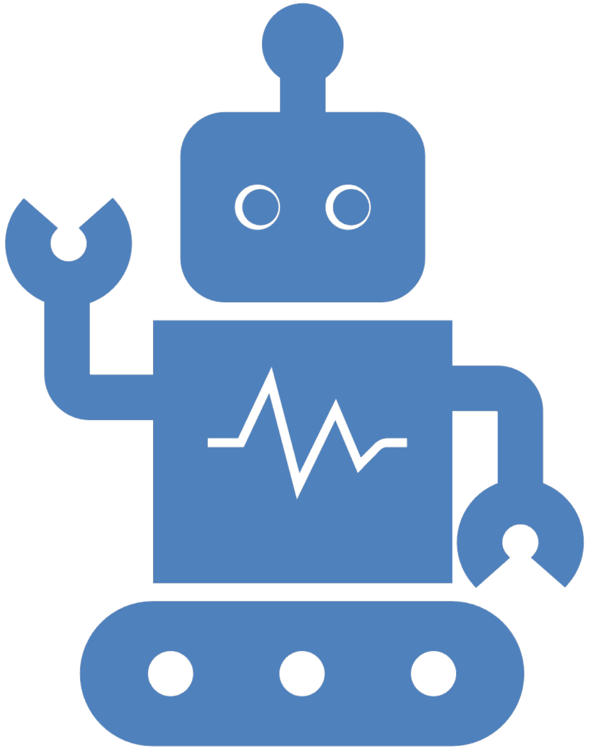
Complementarity → Robustness

The edge of data-derived

Ticks all boxes: “**compute, modeling, human**”

Simplified systematics treatment

Automation

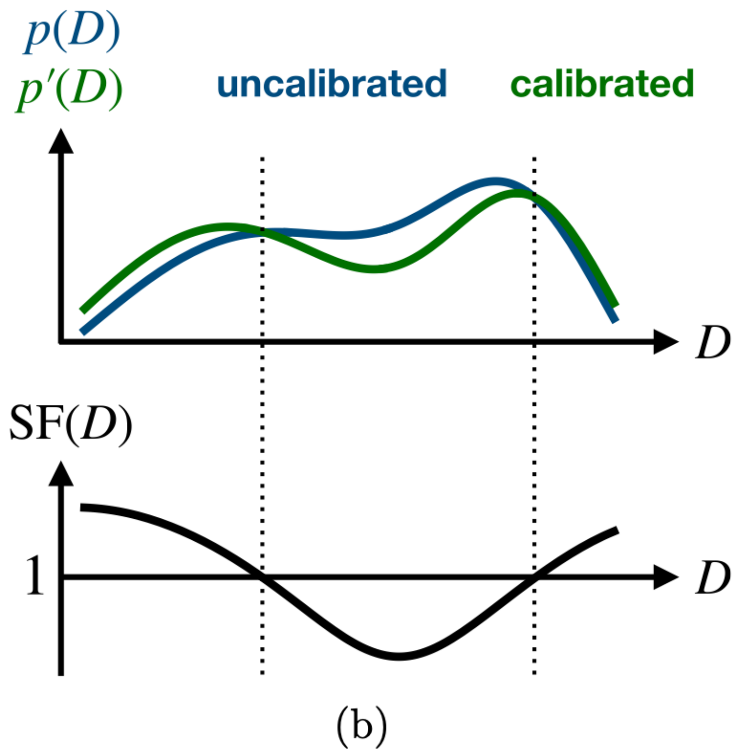


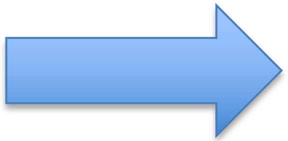
The next level of MC corrections

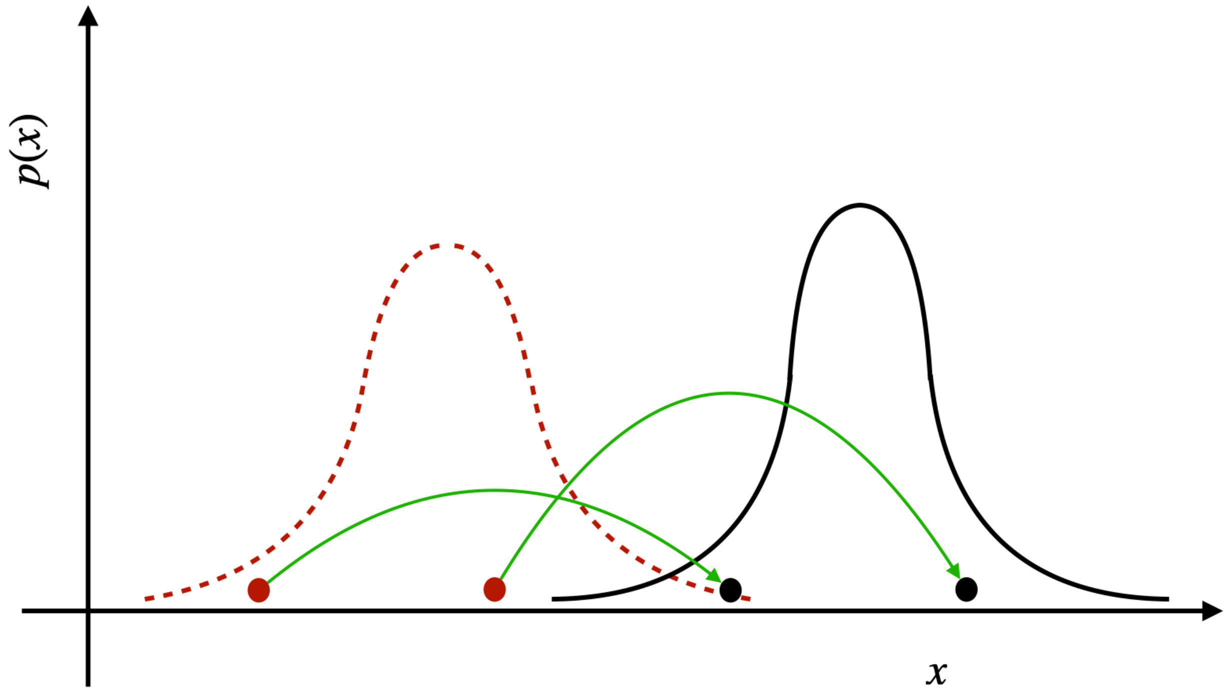
Feed smart corrections back to our theory models

Transport your problems away

Calibrating stochastic simulations with optimal transport







[2107.08648]

The 5th paradigm of scientific discovery

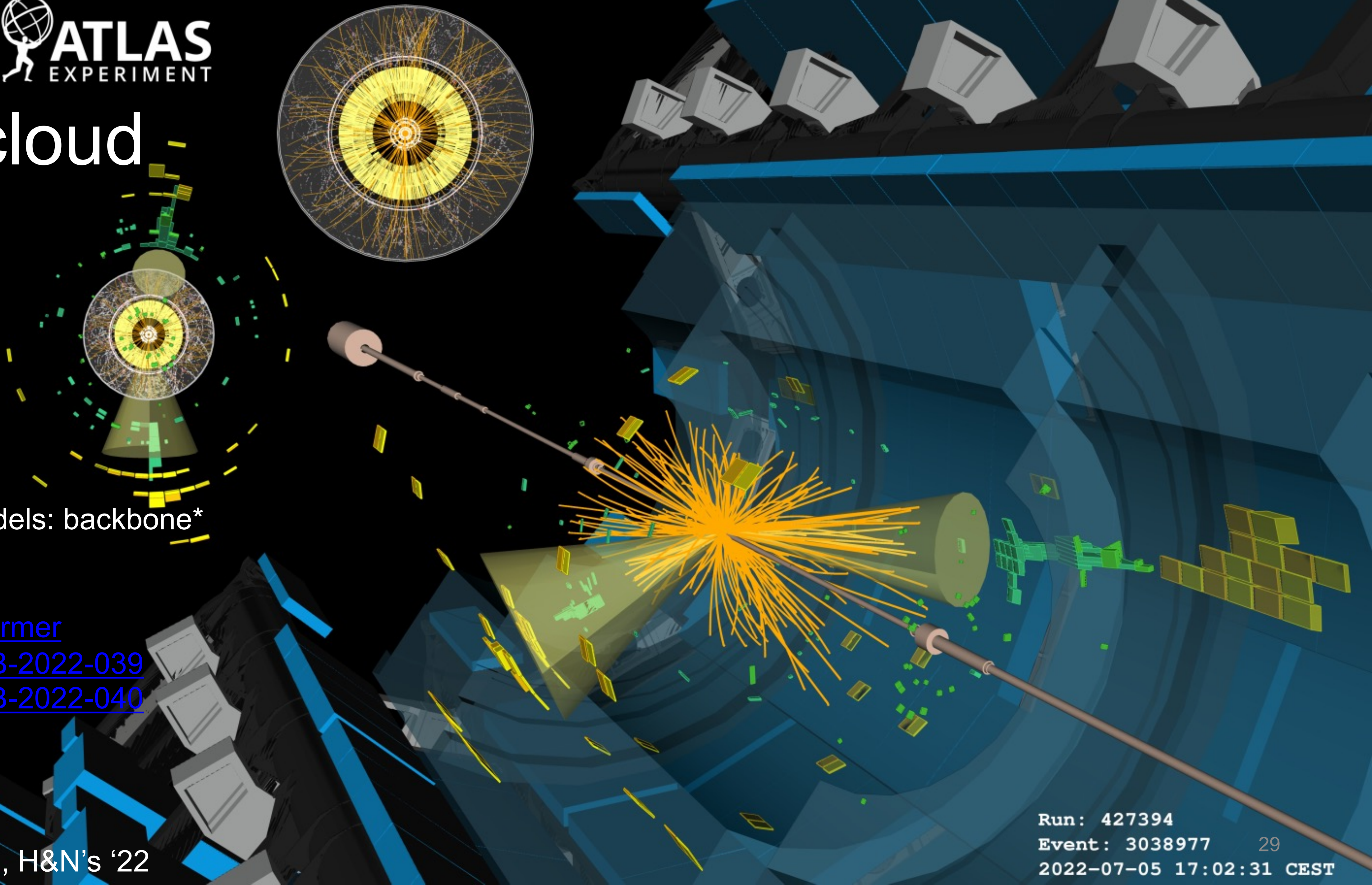
- Simulators: costly, non-differentiable

- (*Local/modular*) surrogate simulators*
  - Fast & differentiable
  - Incorporate inductive bias
  - Anomaly detection, optimisation, design, inference,…

*This finally just came out 2210.06204

Looks like a

point cloud



GNN
Transformers
Foundation models: backbone*
PFN
ParticleNet
Particle Transformer
ATL-PHYS-PUB-2022-039
ATL-PHYS-PUB-2022-040

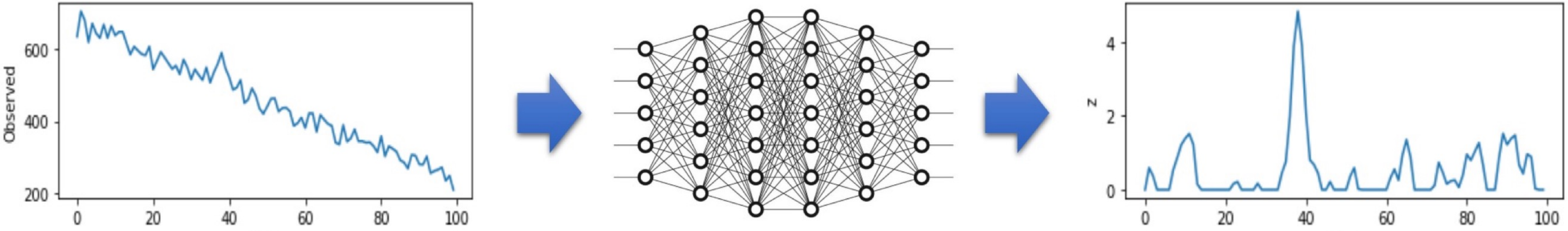
*Lukas Heinrich, H&N's '22

Variation on *typical* bump hunt

Regression:

Mass distribution

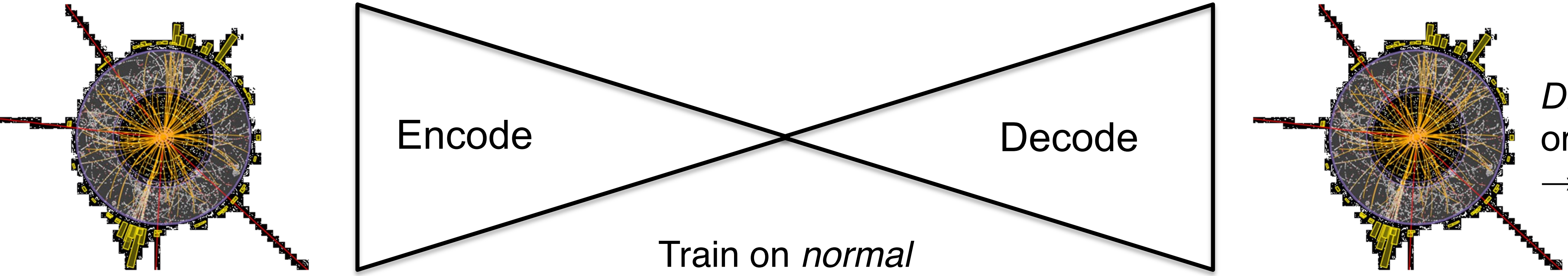
p-value distribution



Challenges: training, validation, out of domain etc.

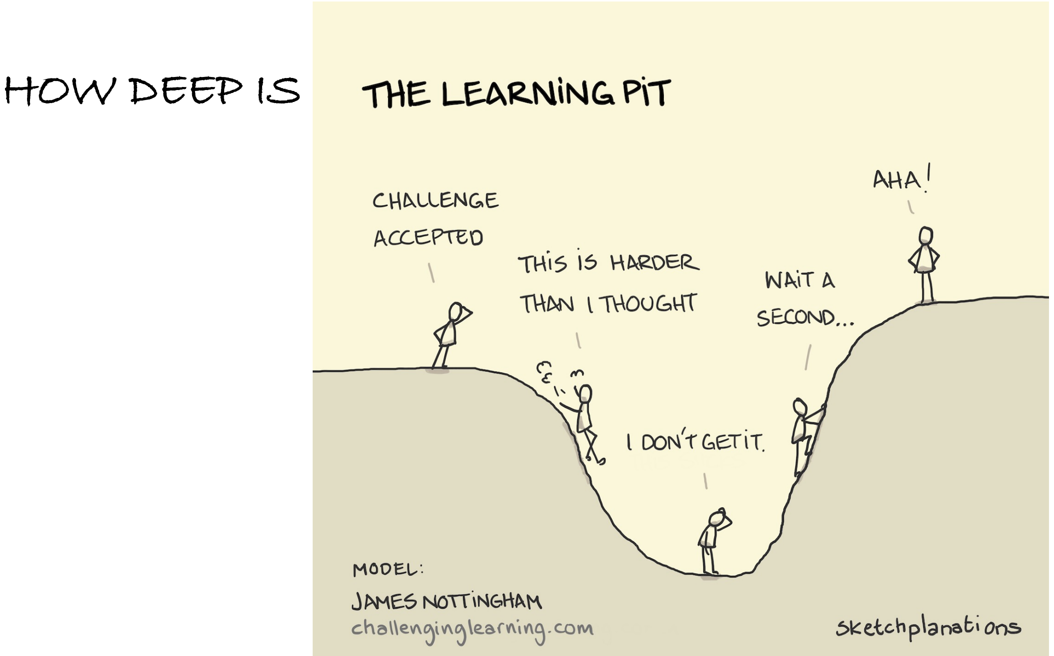
[2107.11573]

Fabulous idea: VAE-based outlier detection



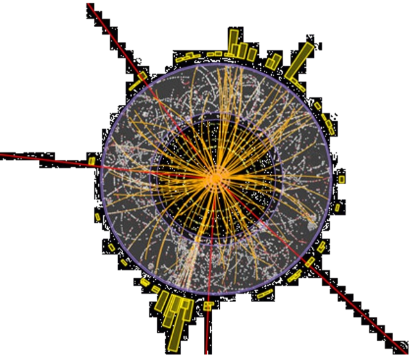
Distance
original – reconstructed
→ anomaly metric

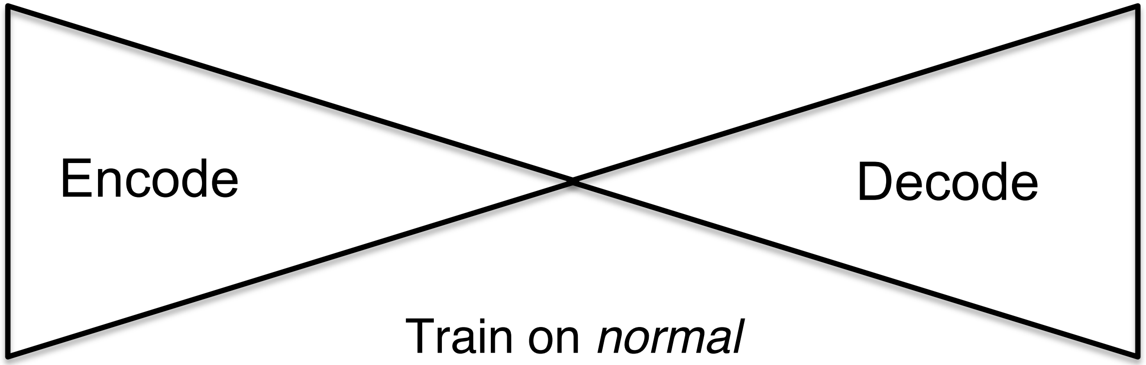
Is it working?

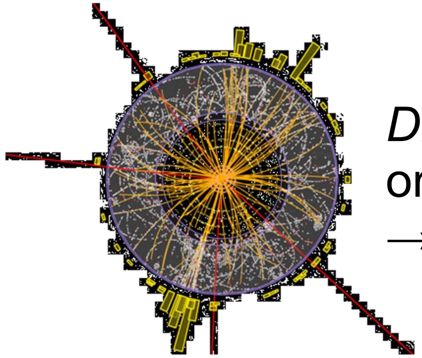


[many references… extend to trigger]

Fabulous idea: VAE-based outlier detection







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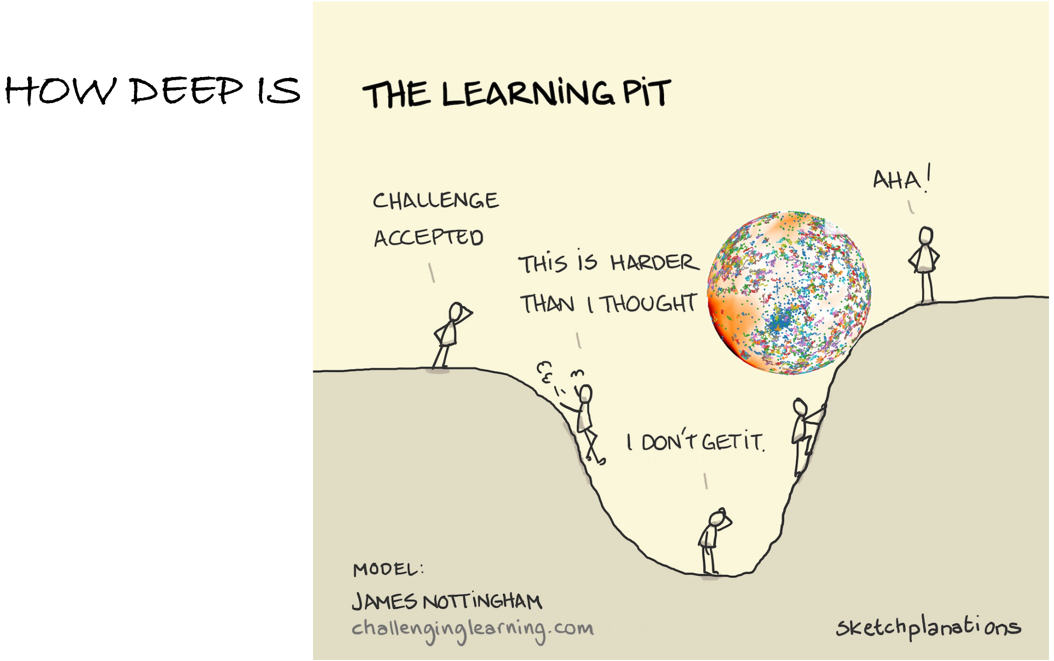


[NAE]

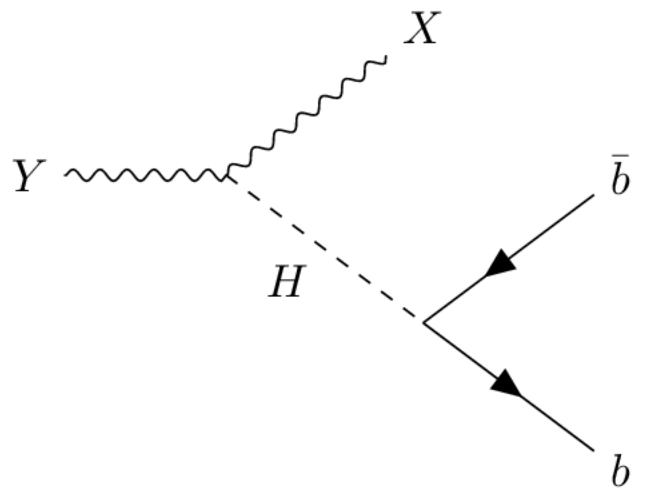
[many references… extend to trigger]

The *add-on* anomaly search

For any standard search

Add *anomaly* signal region*

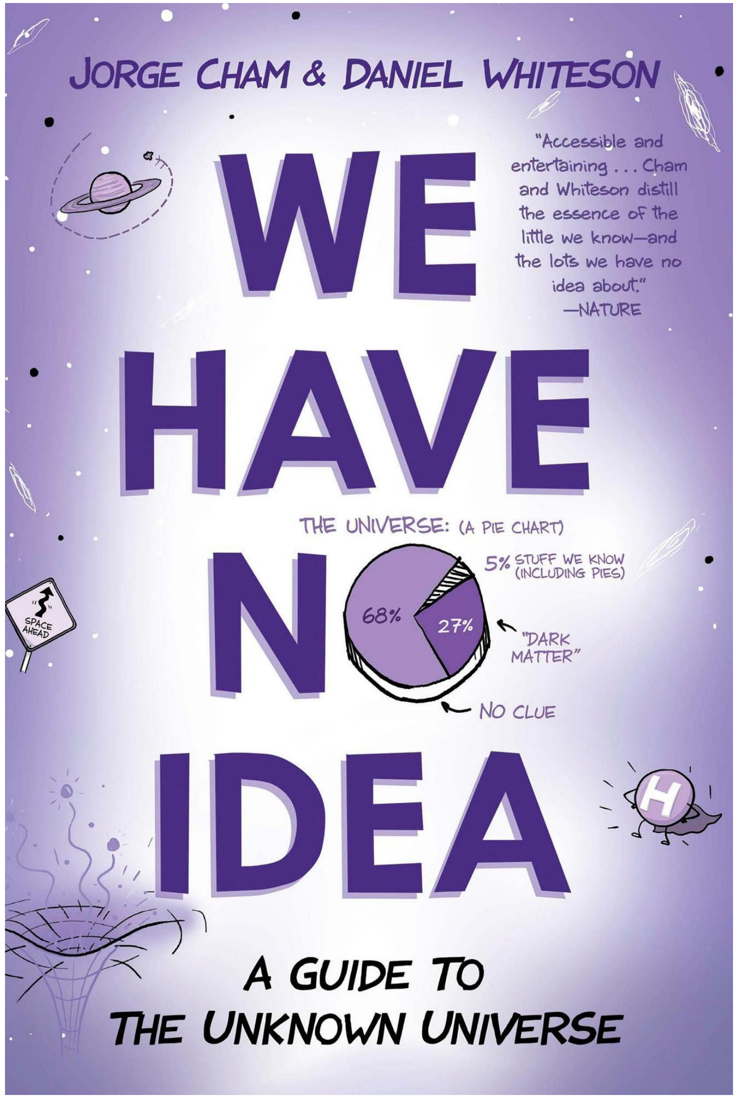
Comes *for free*



[ATLAS-CONF-2022-045]

*Sascha Caron

Imagine we abandon theory guidance



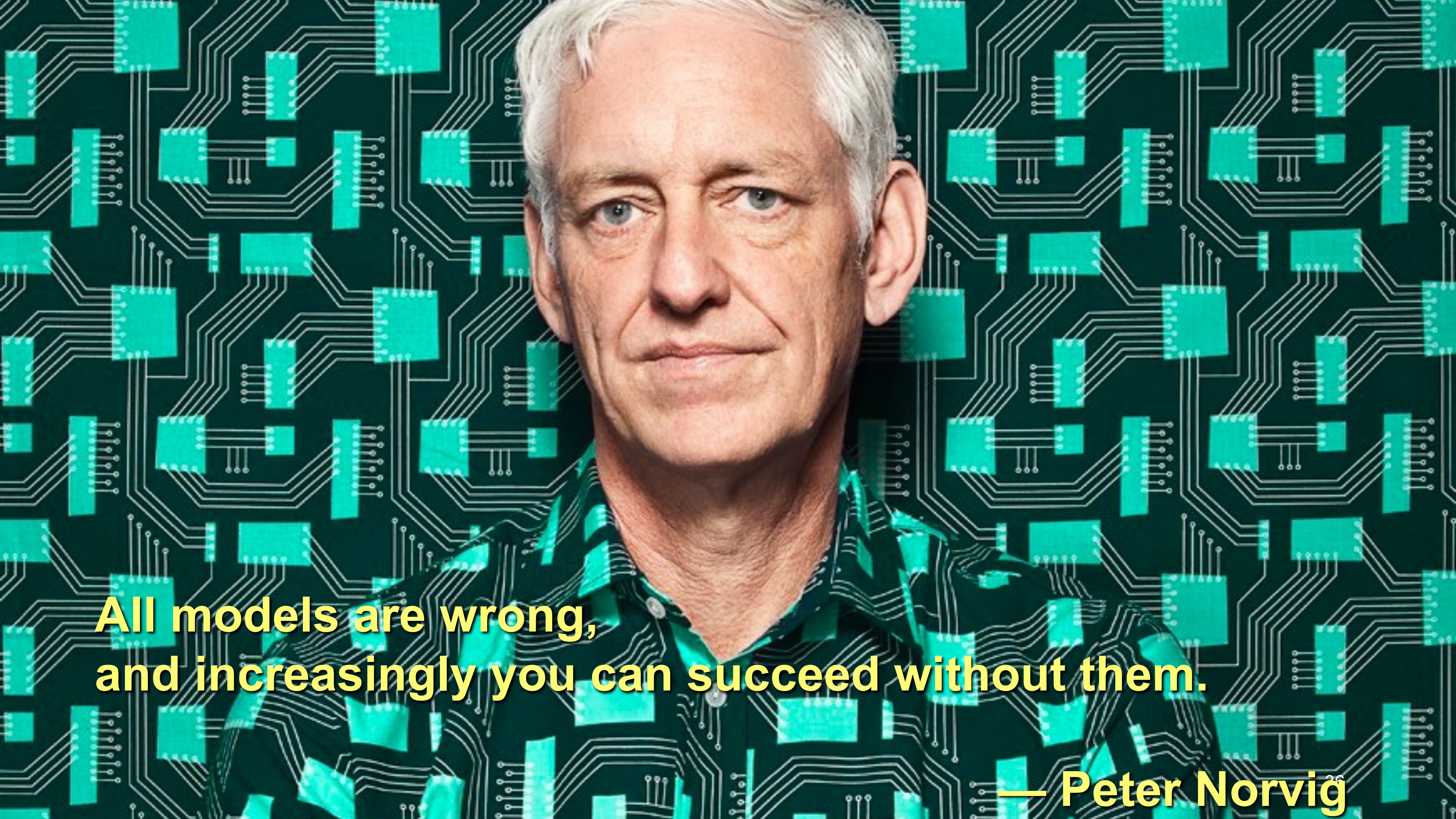
Instead we have an AI oracle

Would we be satisfied?

CHRIS ANDERSON SCIENCE 06.23.08 12:00 PM

THE END OF THEORY: THE DATA DELUGE MAKES THE SCIENTIFIC METHOD OBSOLETE

[Some slides by Kyle Cranmer @ Hammers and Nails ’22]


All models are wrong,
and increasingly you can succeed without them.
— Peter Norvig

Philosophy of Science

What is scientific understanding?

All models are wrong, but some are are useful.

– GEORGE BOX

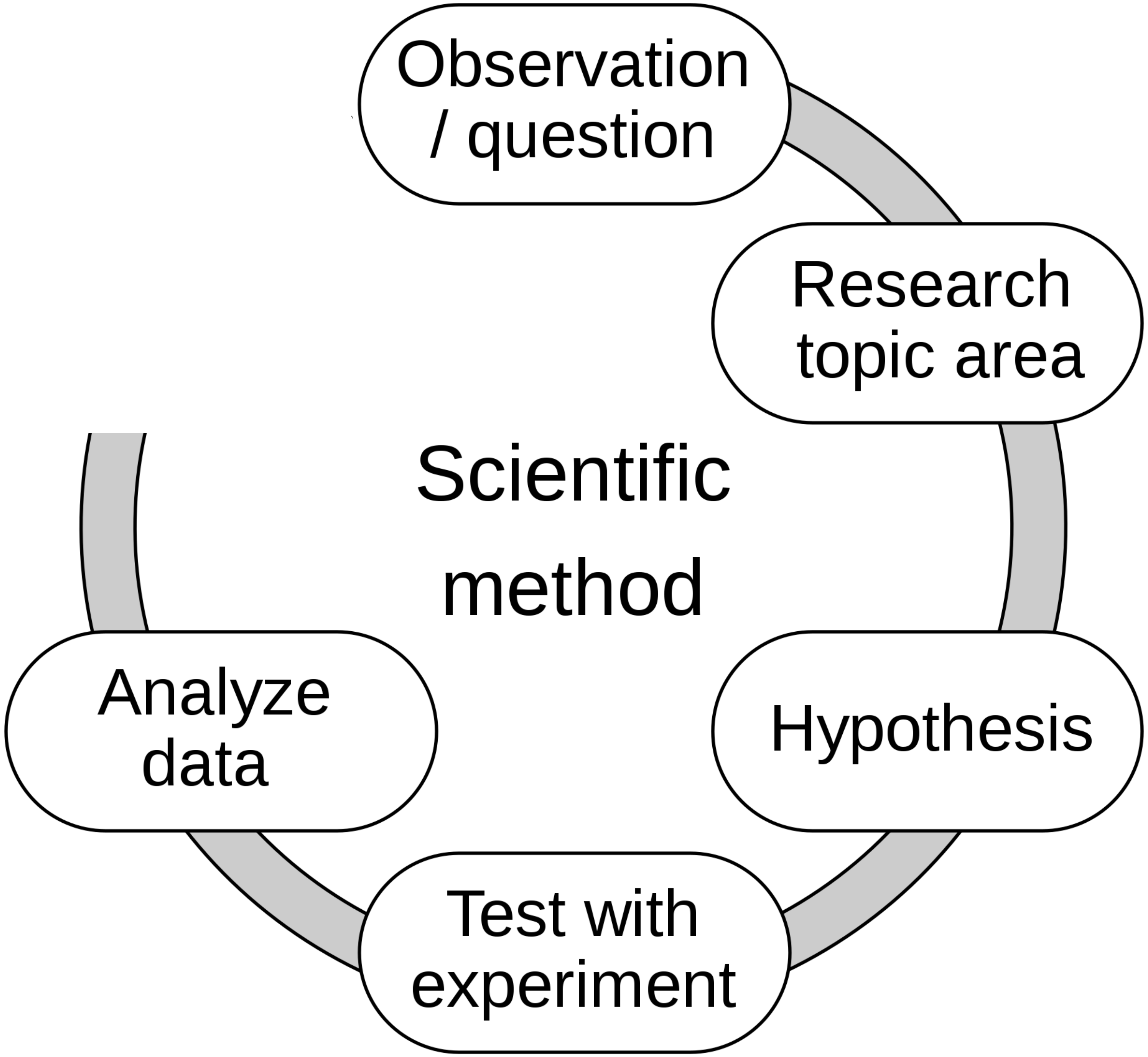
Inject domain knowledge into ML system

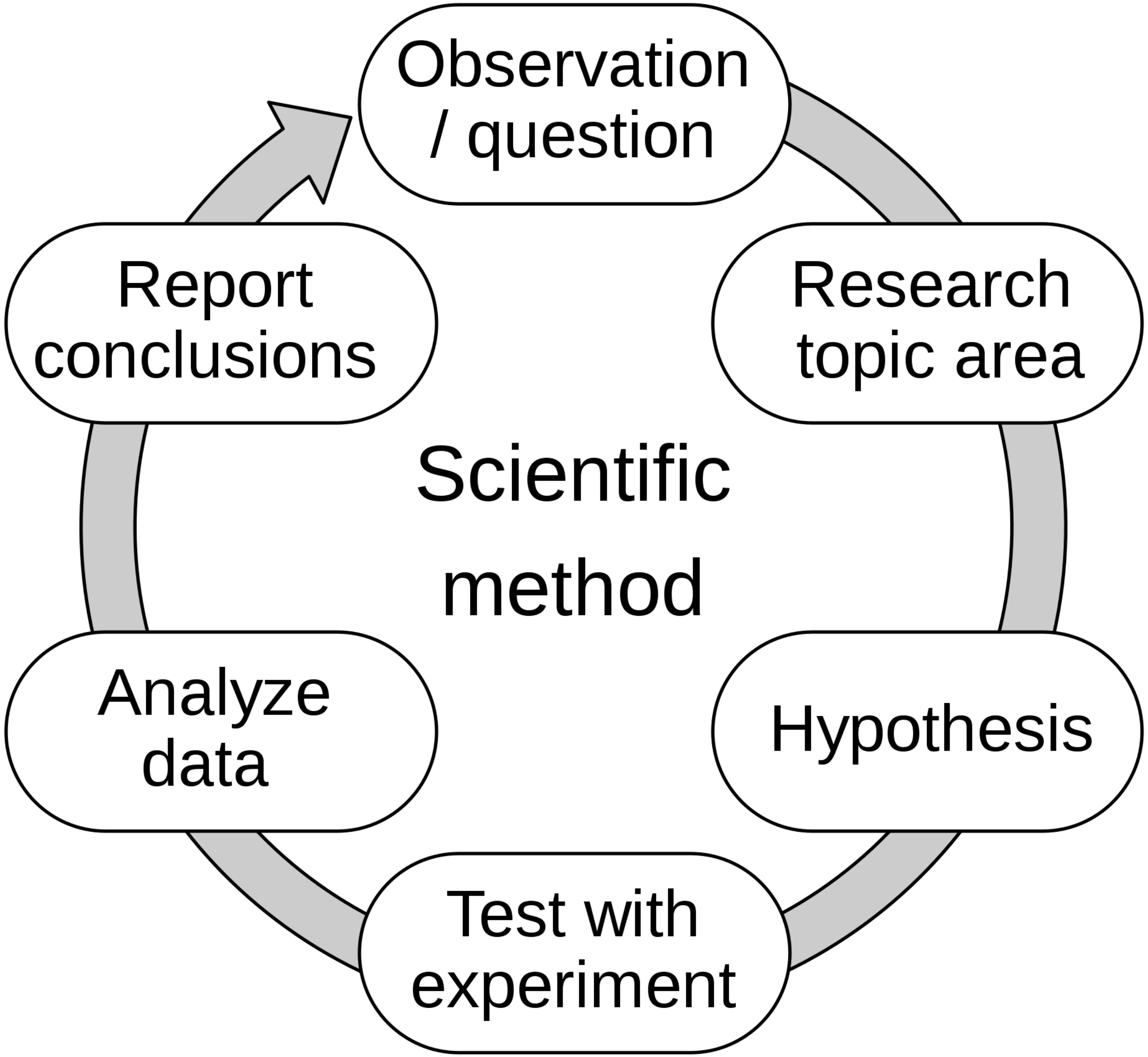
- BSM priors:
  - Crowdsource theorists
  - Generative models
  - …
- Differentiable programing*
- *End-to-end systems*

*Lukas Heinrich, H&N's '22

№ 1 Priority

Maximize
Discovery
Potential

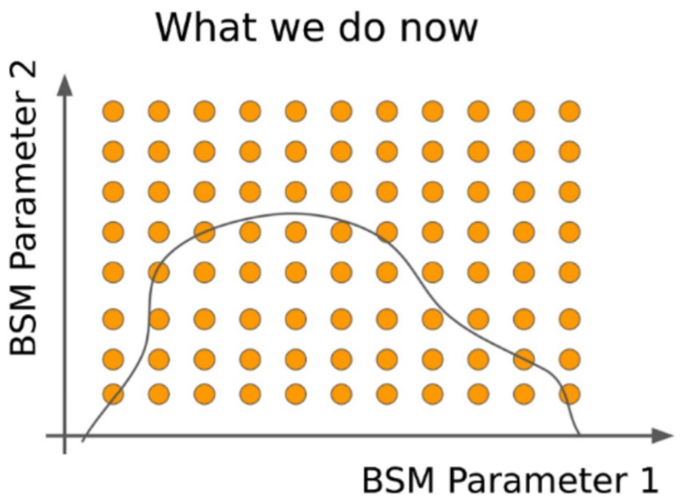

Observation / question
Research topic area
Hypothesis
Test with experiment
Analyze data
Scientific method

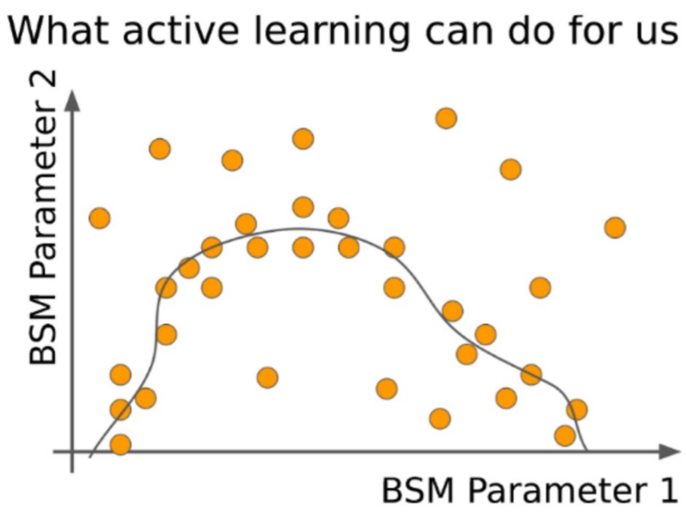

Observation / question
Research topic area
Hypothesis
Test with experiment
Analyze data
Report conclusions
Scientific method

№ 2

(Re)Interpret Results

Smart sampling with active learning



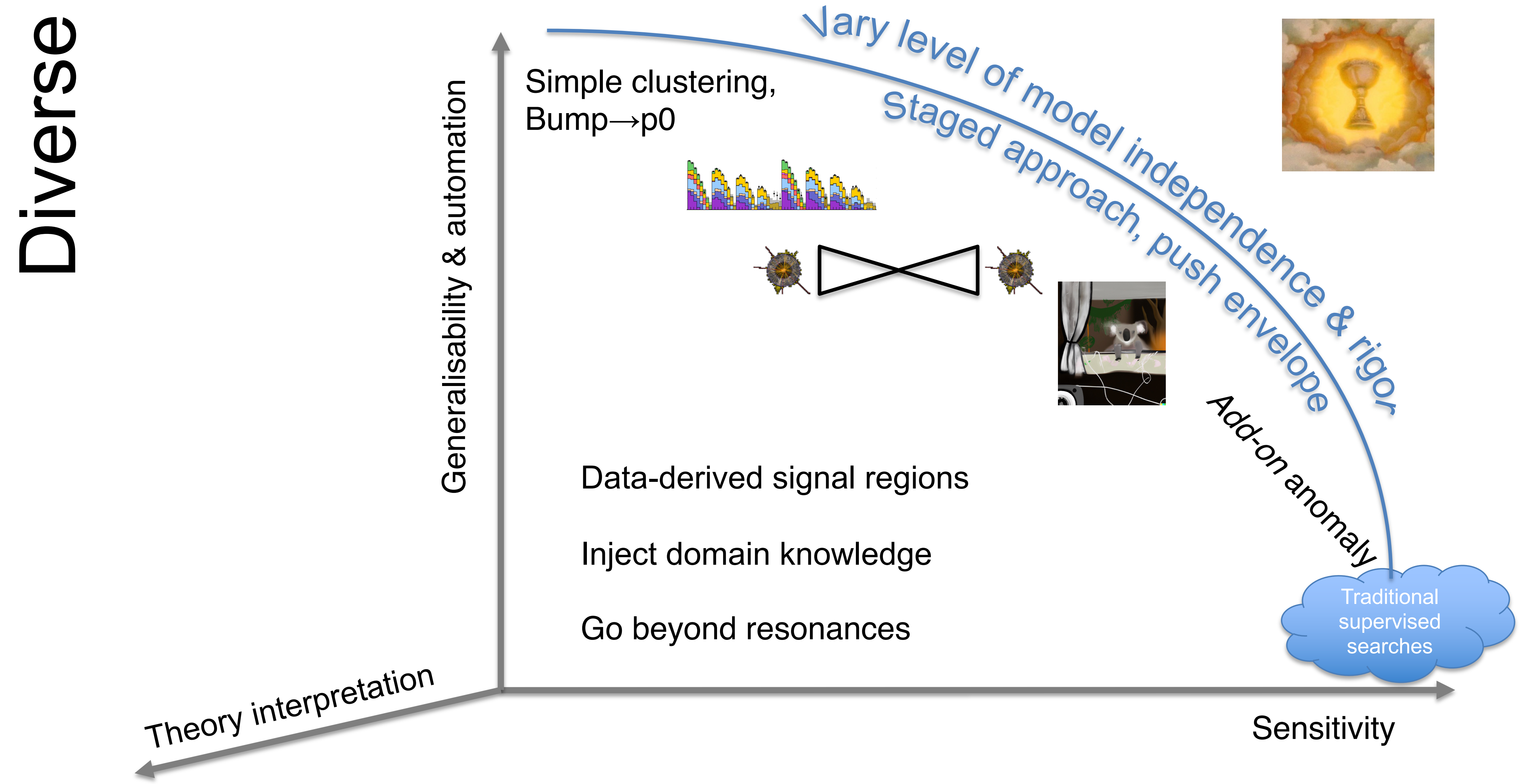


Thrives on high-dimensional theory space

→ Simulate on demand

[Regress on upper limit with GP for ATLAS mono-H(bb) search, ACAT22, ATL-PHYS-PUB-2022-XXX]

Search Strategy

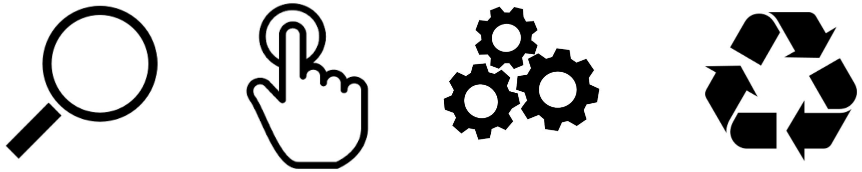


Device Strategy in Experiment

"There is no power for change greater than a community discovering what it cares about."

[Margaret Wheatley]

Be Findable Accessible Interoperable Reusable



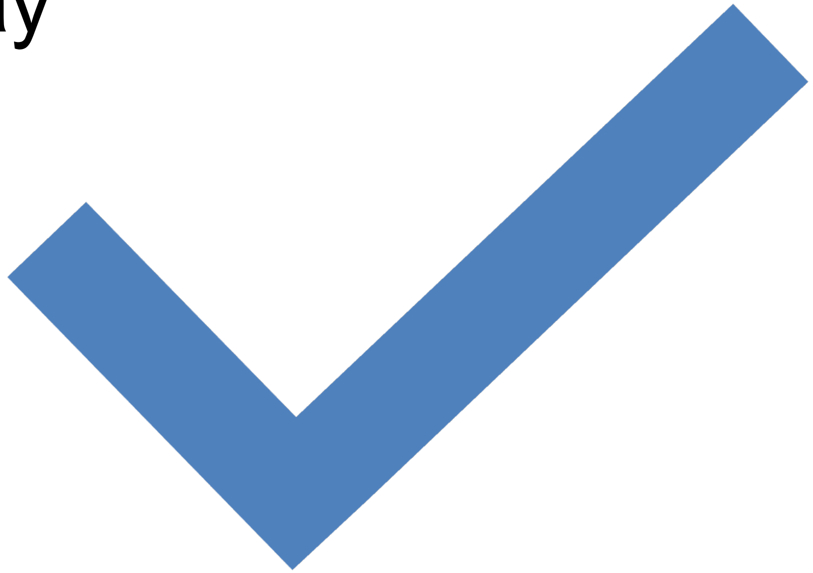
Reusable & differentiable code [e.g. ACTS] → Geant4,…

Common benchmarks, metrics, staged, ceiling analysis,…

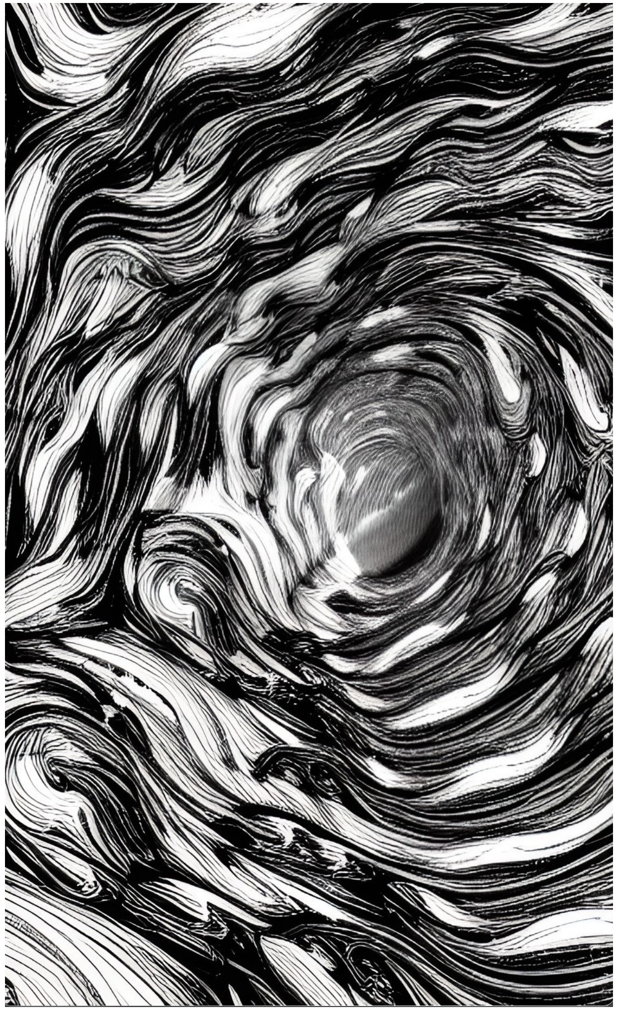
Known knowns

Proof of concepts are *easy*

Production-readiness is hard → Delay



Experiments buy into ML ☺



Brain drain

ML@HEP ↔ *Open Science* @ Experiment

Recognition

Experiment time scale ↔ Fast-moving ML

Fixes?

Fast-track limited-author method papers

Experiments could be **the** MNISTs

Would speed up production readiness

And of course ML4Jets !

Concluding remarks

HEP evolves

ML is one of our sharpest tools

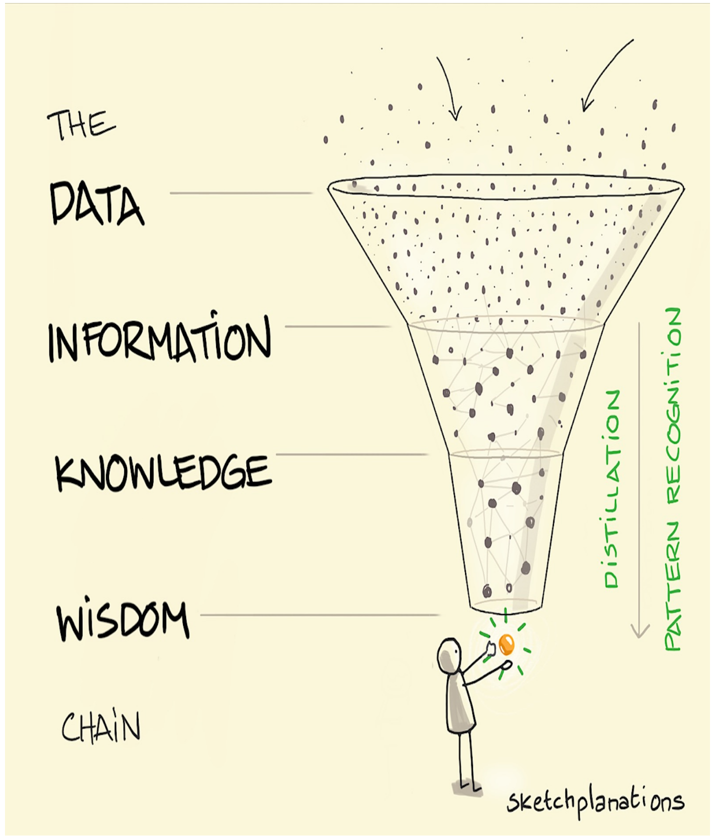
Tackle Big Goals as a Community

Value human resources → automation with ML

Concept → production

New *diverse* search strategy

Need all you bright young ML4Jets minds !



ATLAS EXPERIMENT

syn·er·gy | ˈsinərjē |

UNIVERSITÉ DE GENÈVE
FACULTY OF SCIENCE

PIs


TG


Slava Voloshynovskiy


François Fleuret

PhD students


Tomke Schröer


Malte Algren


Lukas Ehrke


Matthew Leigh


Debajyoti Sengupta


Sam Klein


Guillaume Quétant


Mariia Drozdova


Ivan Oleksiyuk


Bálint Máté


Atul Kumar Sinha


Daniele Paliotta

postdocs


Knut Zoch


Manuel Guth


Johnny Raine

This could be you !


Olga Taran

Full spectrum: physics - CS

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Alexander von Humboldt Stiftung / Foundation

Swiss National Science Foundation

Sinergia

Swiss Government Excellence Scholarships
STUDY IN SWITZERLAND

ATLAS EXPERIMENT

syn·er·gy | ˈsinərjē |

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Slava Voloshynovskiy

François Fleuret

PhD students

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Matthew Leigh

Debajyoti Sengupta

Sam Klein

Guillaume Quétant

Mariia Drozdova

Ivan Oleksiyuk

Bálint Máté

Atul Kumar Sinha

Daniele Paliotta

postdocs

Knut Zoch

Manuel Guth

Johnny Raine

This could be you !

Olga Taran

Full spectrum: physics - CS

This could be you !

Contact Tobias.Golling@unige.ch

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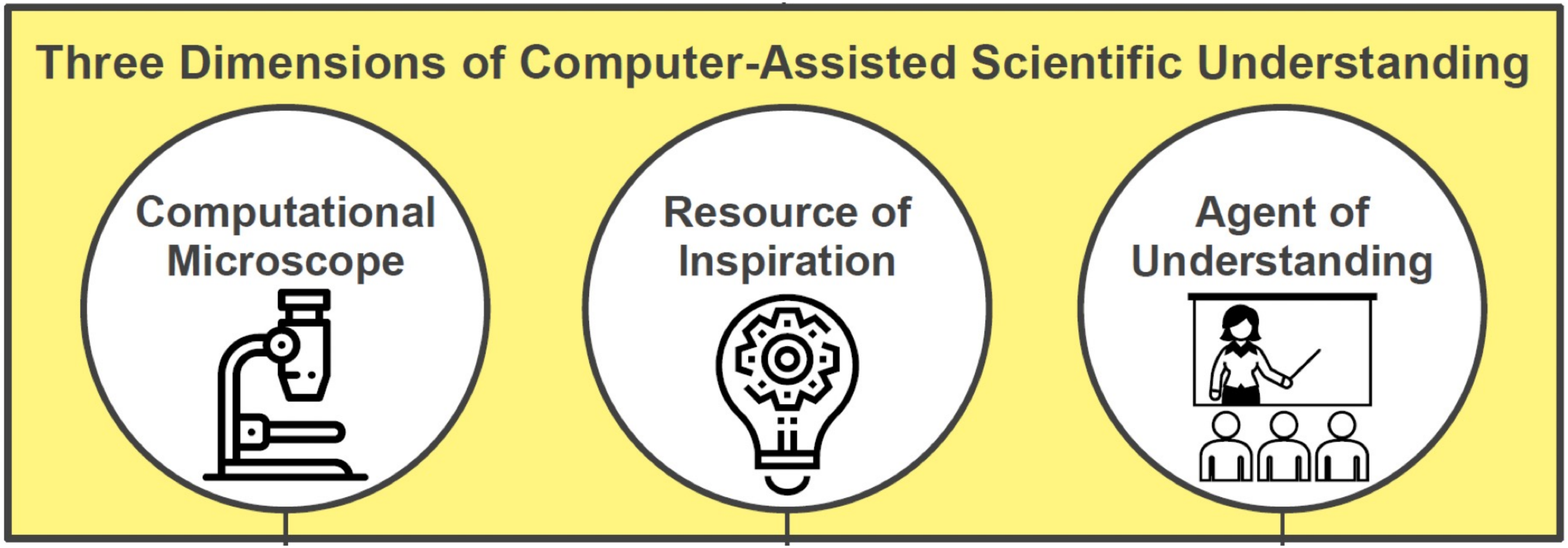
Sinergia

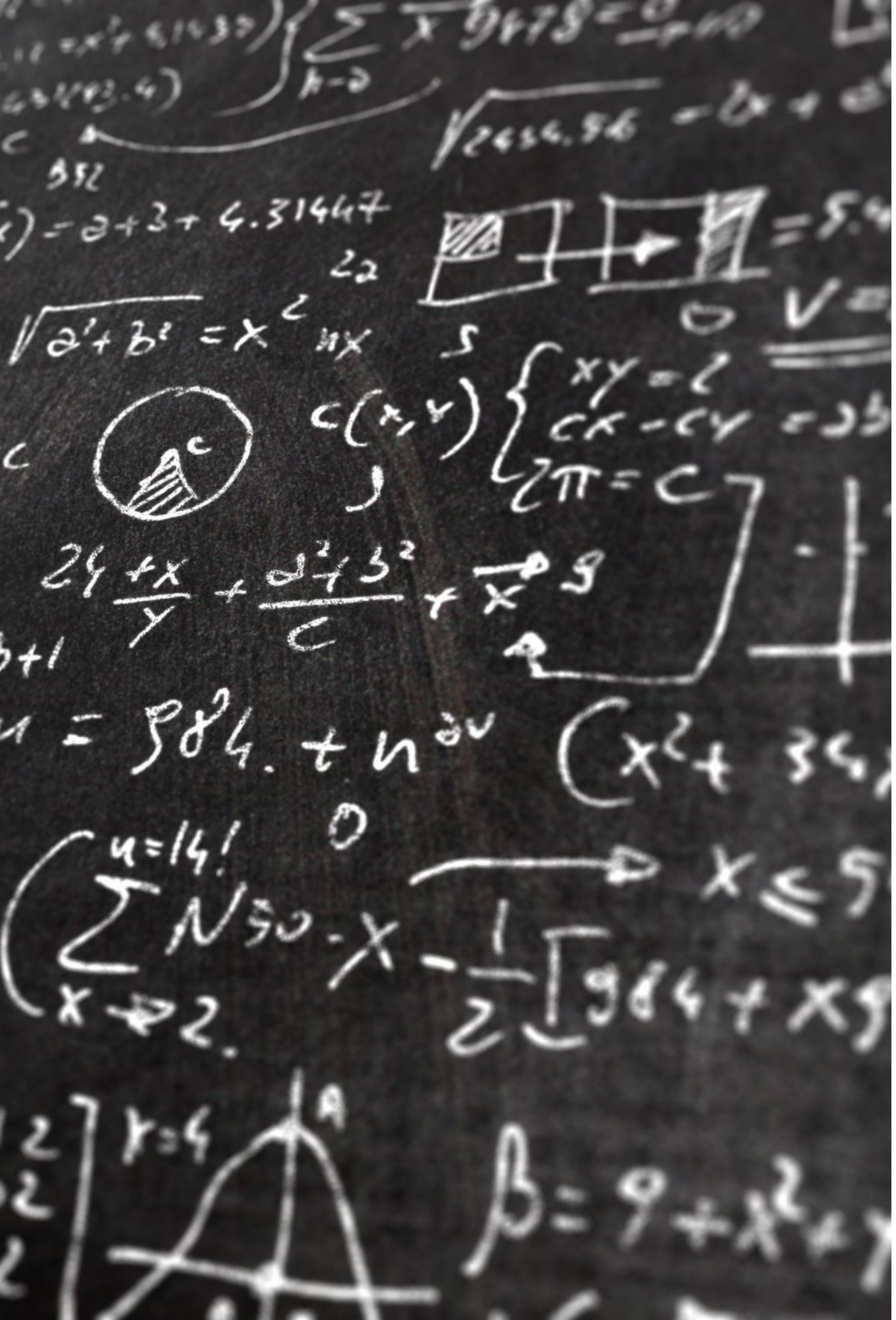
Swiss Government Excellence Scholarships
STUDY IN SWITZERLAND

Backup

Qualitative change

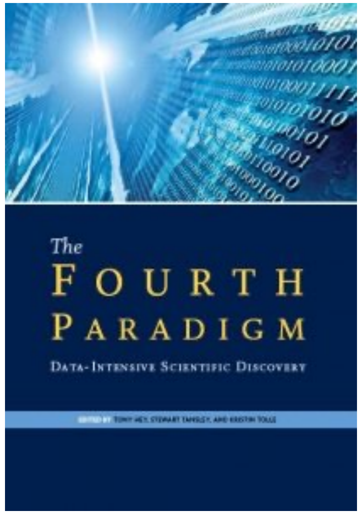


[Mario Krenn, et. al. 2204.01467]



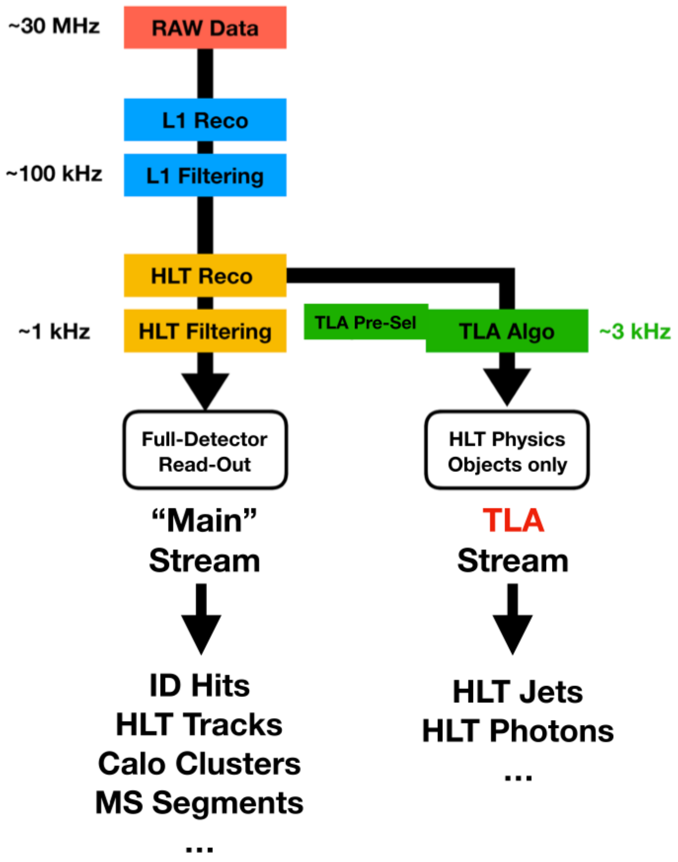
The 4 paradigms of scientific discovery

1. Observation of natural phenomena
2. Theoretical models of nature
3. Numerical computation
4. Data-intensive scientific discovery



Jim Gray

TLA



Physics main

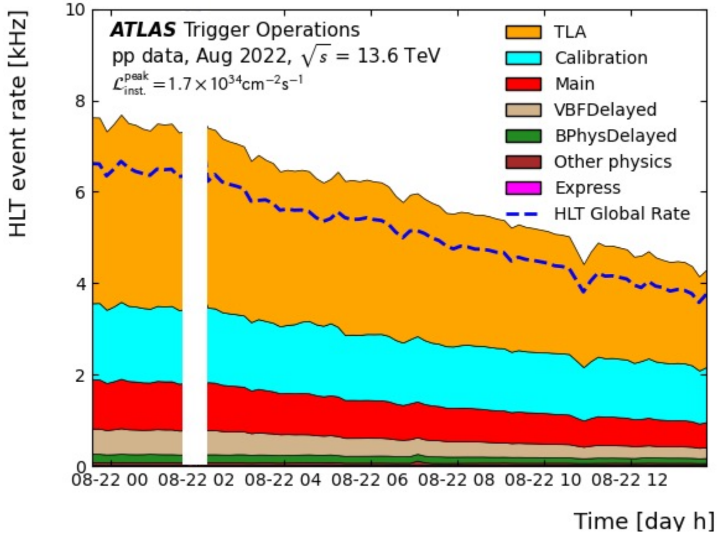
$\sim 1\ \text{kHz} \times 1.5\ \text{MB} \rightarrow 1.5\ \text{GB/s}$

TLA

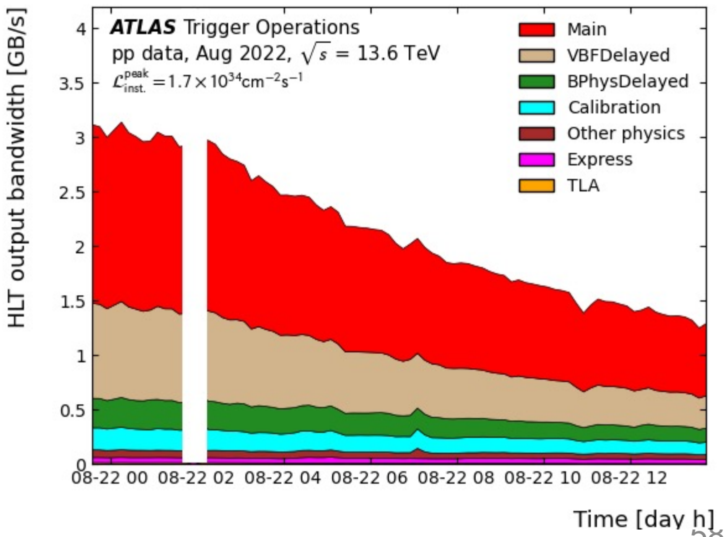
$\sim 4\ \text{kHz} \times 5\ \text{kB} \rightarrow 20\ \text{MB/s}$

- Trade event size for rate!
- Save only HLT objects
- Challenge: calibration!

TLA stream has highest rate...

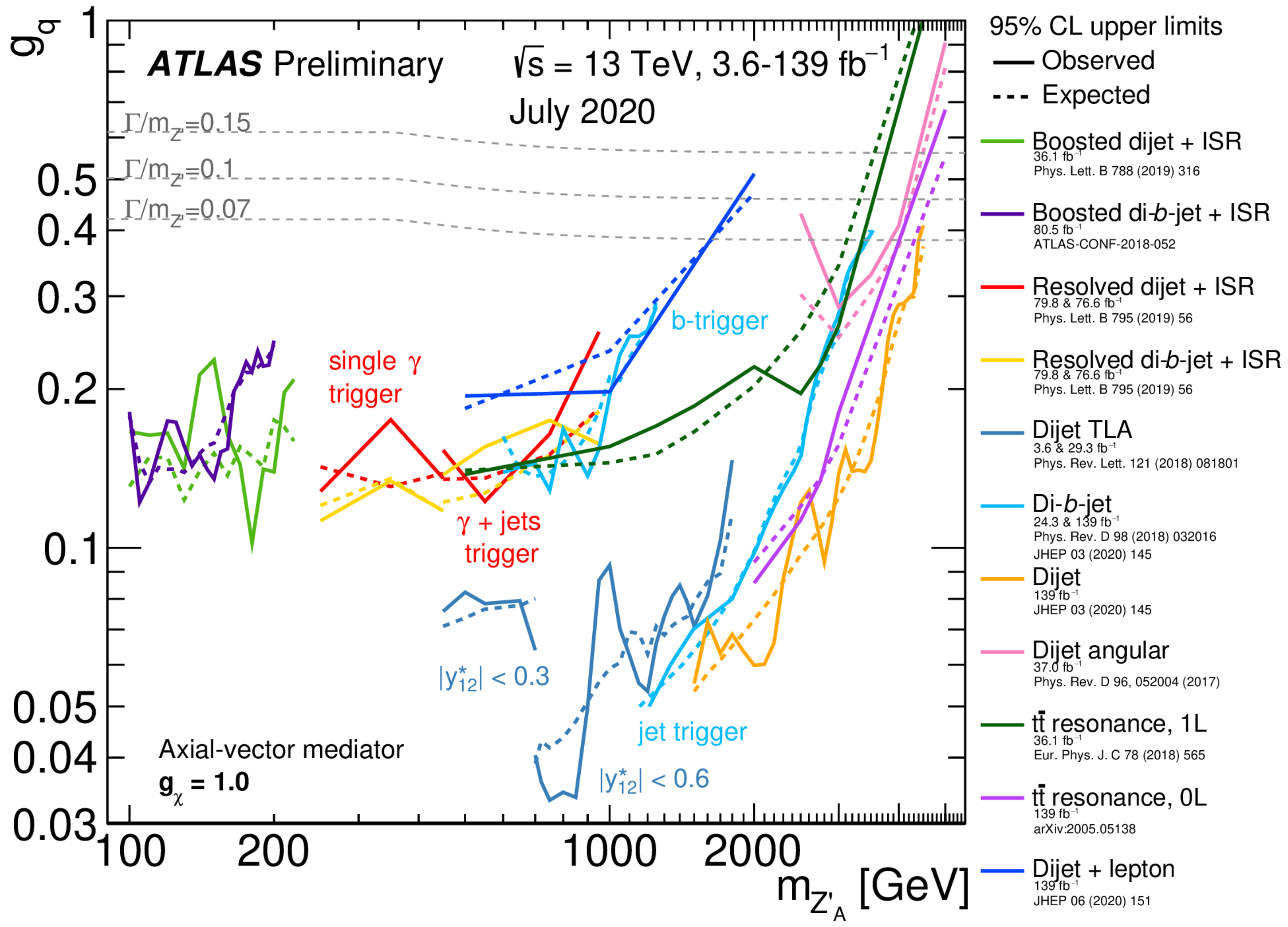


...but lowest bandwidth



[TriggerOperationPublicResults]

BSM@TLA



- Extent search to anomaly@TLA

[CombinedSummaryPlots/EXOTICS]