

Harnessing AI in accelerating rational vaccine design.

Aligning the right tool with the most impactful application

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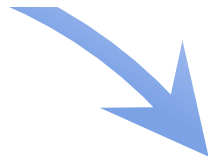
VACCINE AND INFECTIOUS DISEASE ORGANIZATION

VIDO.ORG



Overall computational strategy

Immunogenic antigen



Optimally synergistic adjuvant



Response

Molecular recognition of pathogen; antigen selection

System-wide immune signaling; antigen-adjuvant co-selection for max immune memory

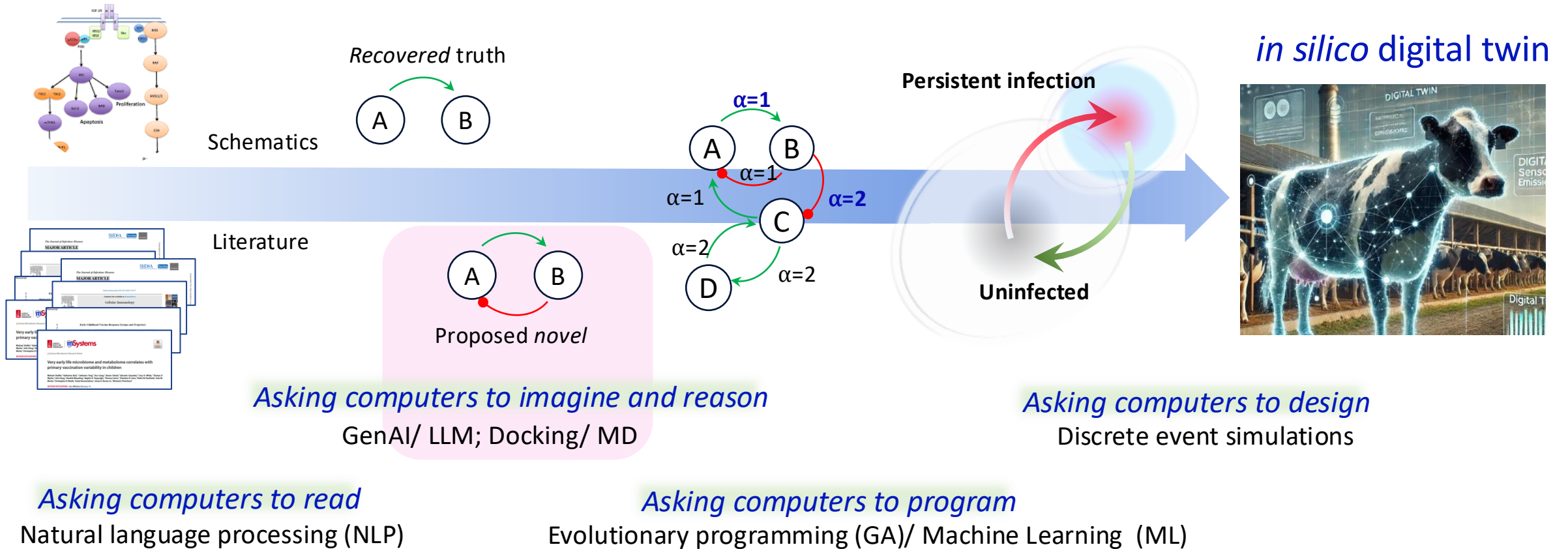
Knowledge-driven assembly of a digital twin

(a) The right pieces

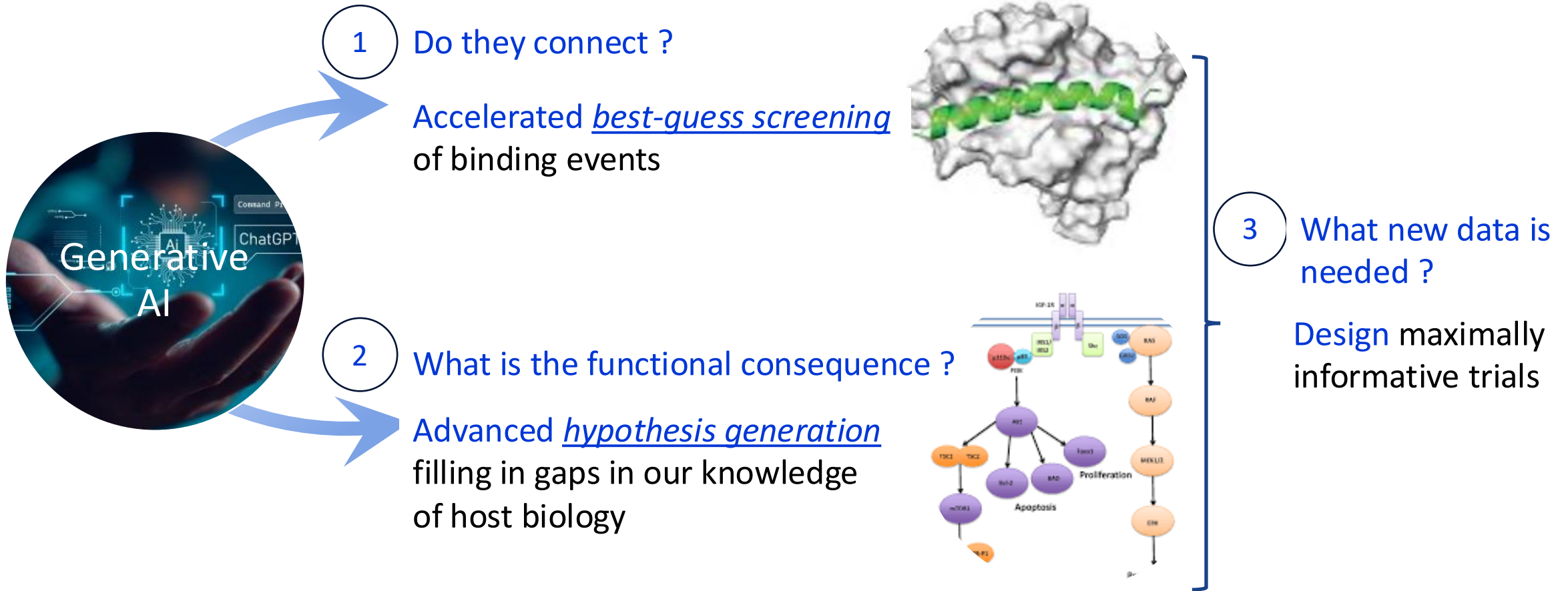
(b) Connecting the dots

(c) Explaining what I see

(d) Collecting *insightful* data



Connecting the dots with AI



What about size

Very large – *very general*

Smaller domain and task-specific

Very compact – *very specific*

Local & highly secure



Llama 3 ~70 Billion parameters
Latest > several Trillion



Tiny BERT ~ 4 Million parameters

Reconstructing Biological Pathways by Applying Selective Incremental Learning to (Very) Small Language Models

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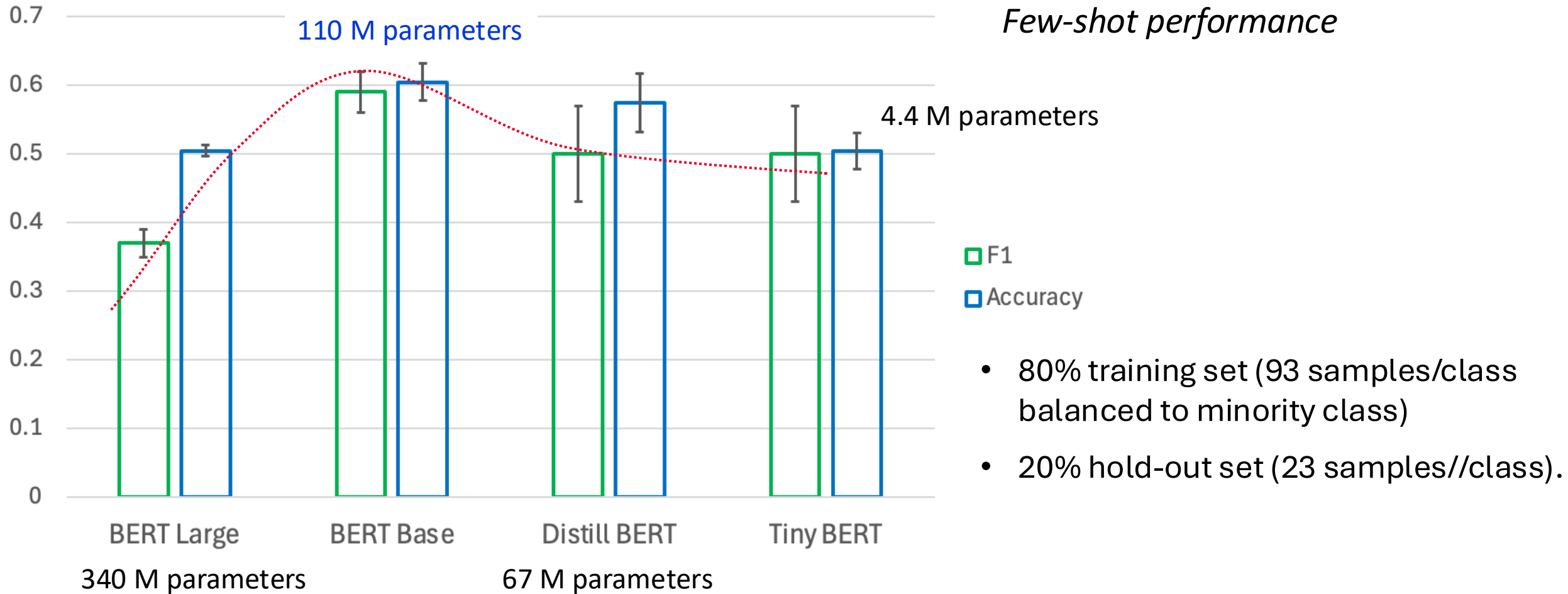
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Mathematical Immunology &
Immunodynamics



Out of the box



Creating a specialist



DeepSeek-R1: Incentivizing Reasoning Capability in LLMs via Reinforcement Learning

DeepSeek-AI
research@deepseek.com



A *selective incremental* learning

- Not all examples are informative or useful
- Partially redundant and/ or unreliable examples can:
 - Introduce **significant bias** that washes out or overshadows informative examples
 - Are hugely **inefficient**, unnecessarily long and **resource-intensive** model fine-tuning
- *High containment data will be sparse, difficult and expensive to acquire*

Guo D, Yang D, Zhang H, Song J, Zhang R, Xu R, Zhu Q, Ma S, Wang P, Bi X, Zhang X.
Deepseek-r1: Incentivizing reasoning capability in LLMs via reinforcement learning. arXiv preprint arXiv:2501.12948. 2025 Jan 22.

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The next most informative example

Conceptual criterion

1. How confident or certain in my guess for this new example?
2. What is the probability that I am guessing correctly

- Randomly (baseline control)
- Least certain; diversity (entropy)
- Largest shift in model (EGL)
- **Label-informed ...Most certain but probably wrong**

Evaluating the Performance of Transformer-based models and ML Strategies for Vaccine Epitope Selection (PRRS)

Aspen Erlandsson Brisebois^{1,2}, Jason Broderick^{1,2}, Zahed Khatooni¹, Heather L. Wilson¹, Sureesh Tikoo¹, Steven Rayan^{3,4}, Gordon Broderick^{1,3,4}

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Reconstructing Biological Pathways by Applying Selective Incremental Learning to (Very) Small Language Models

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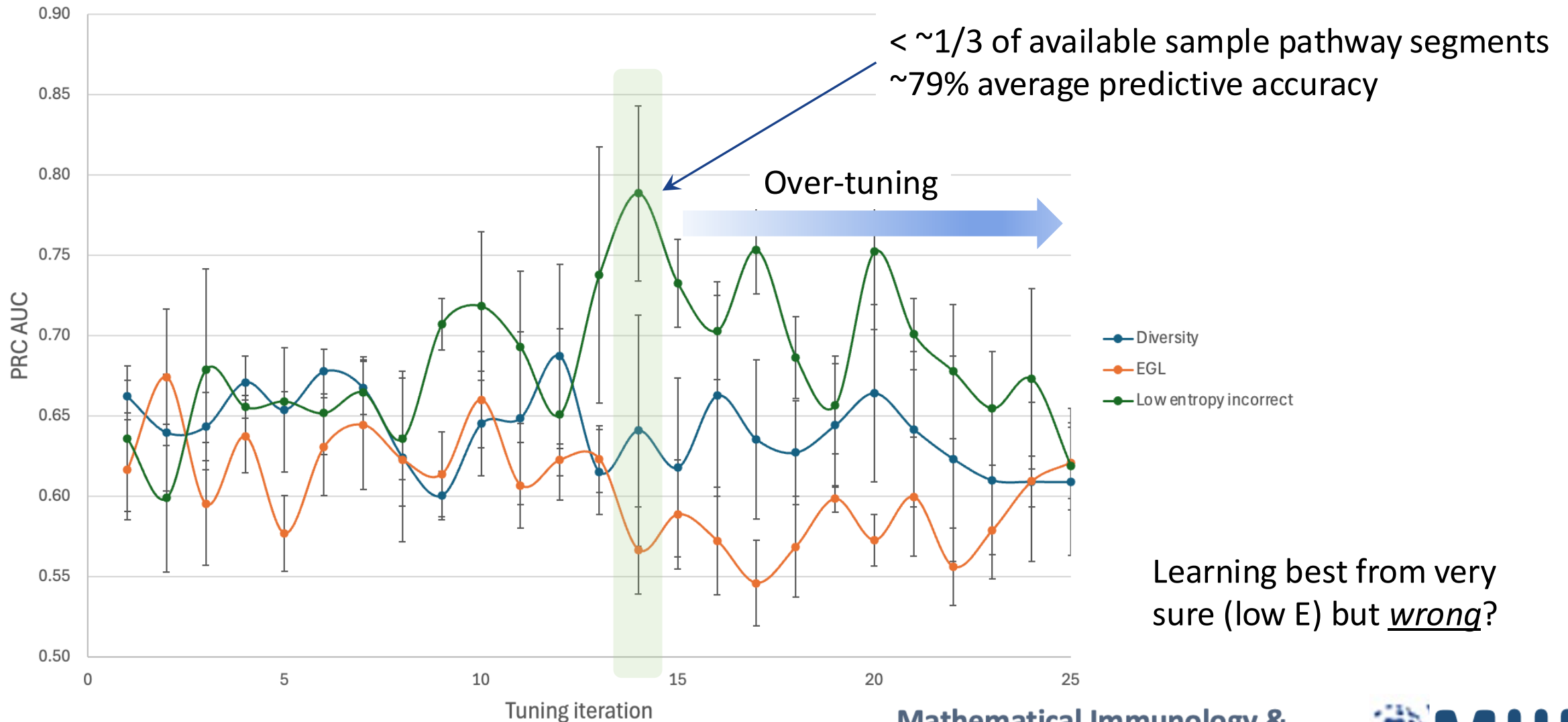
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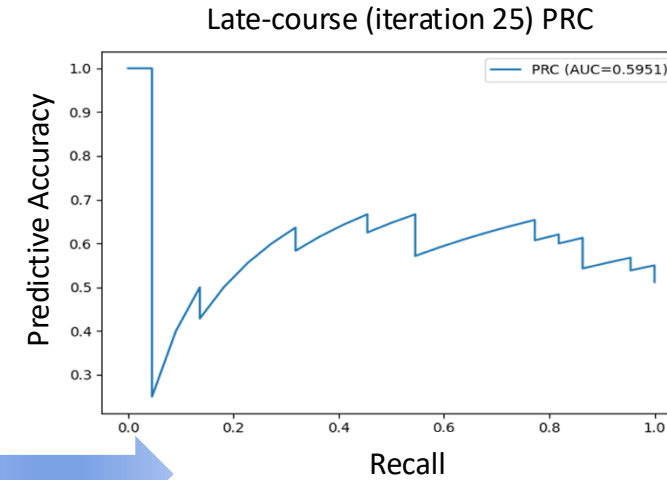
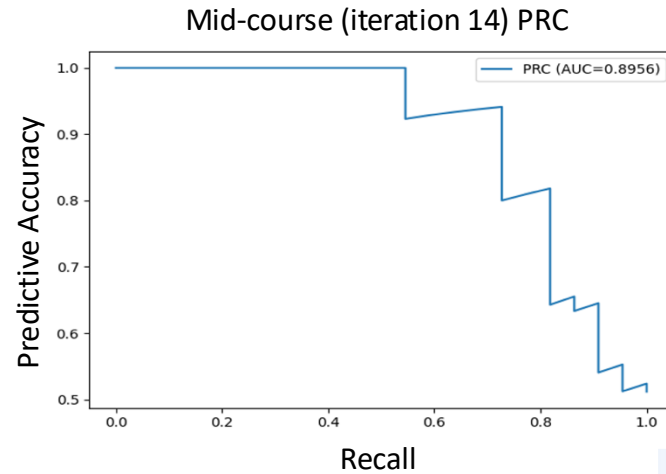
Does protein A regulate protein B?



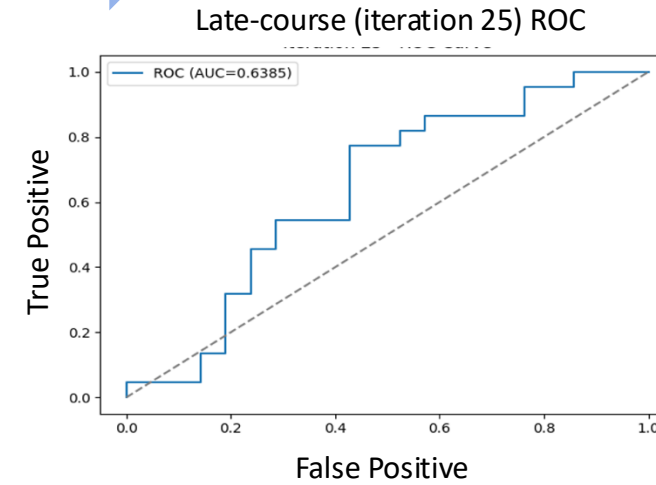
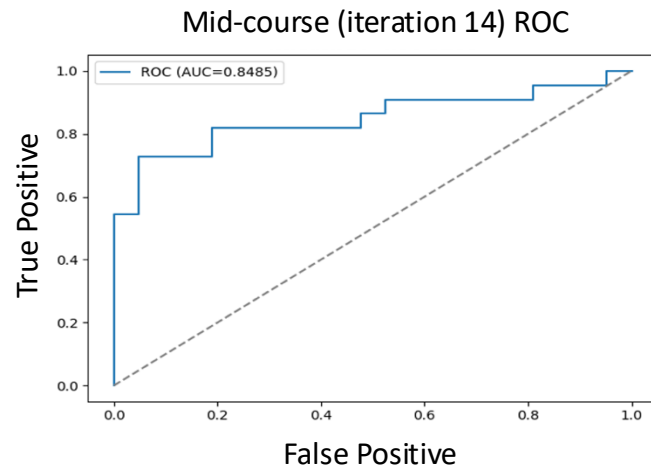
Learning best from very sure (low E) but wrong?

Does protein A regulate protein B?

Low entropy incorrect policy



Over-tuning

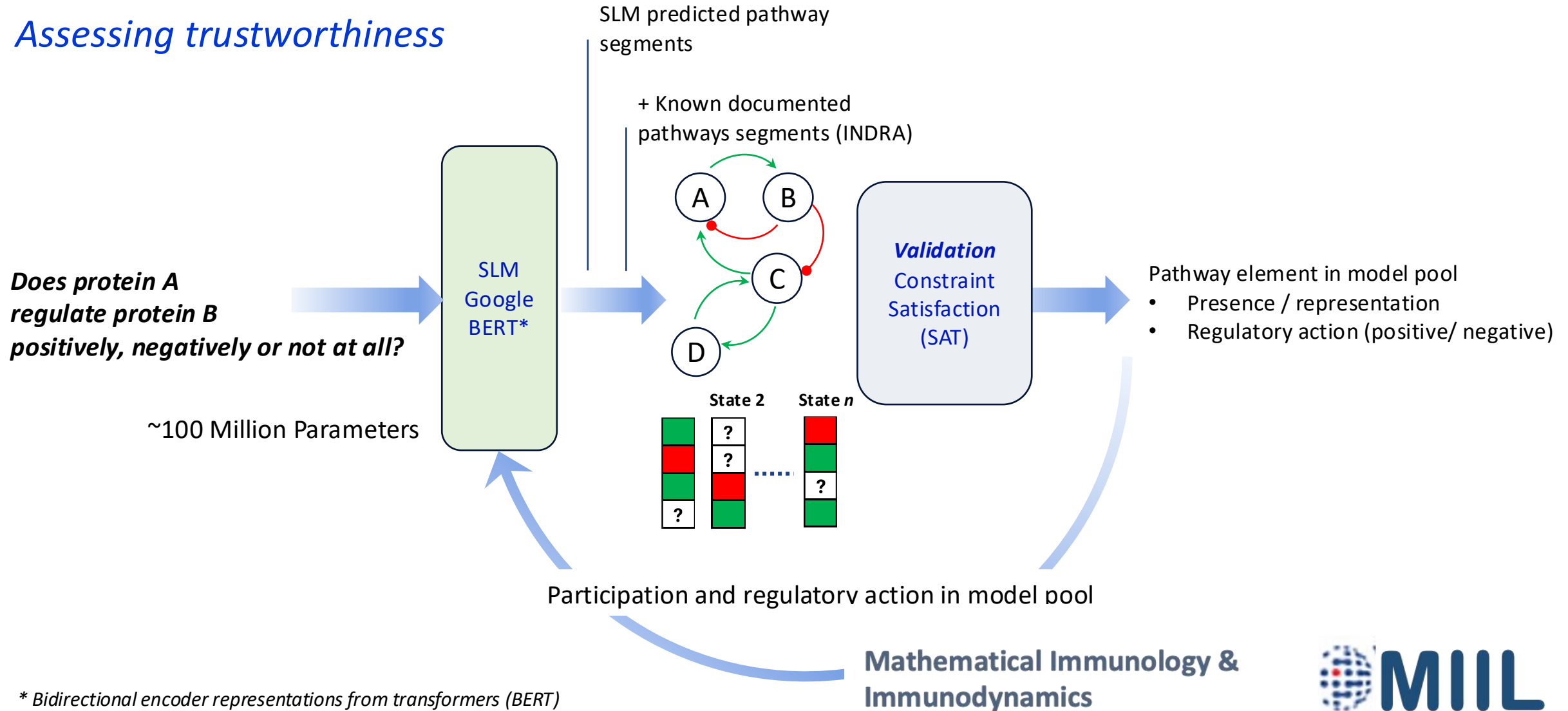


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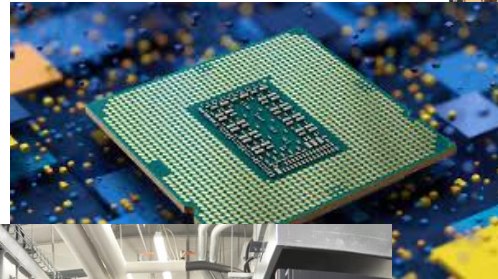
Validation of putative regulation

Assessing trustworthiness

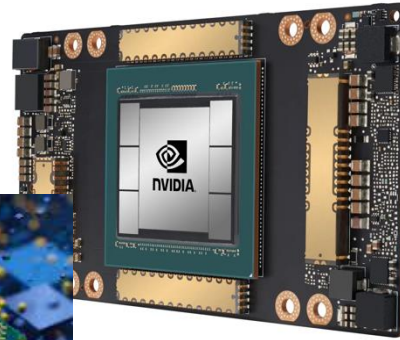


Powering AI models

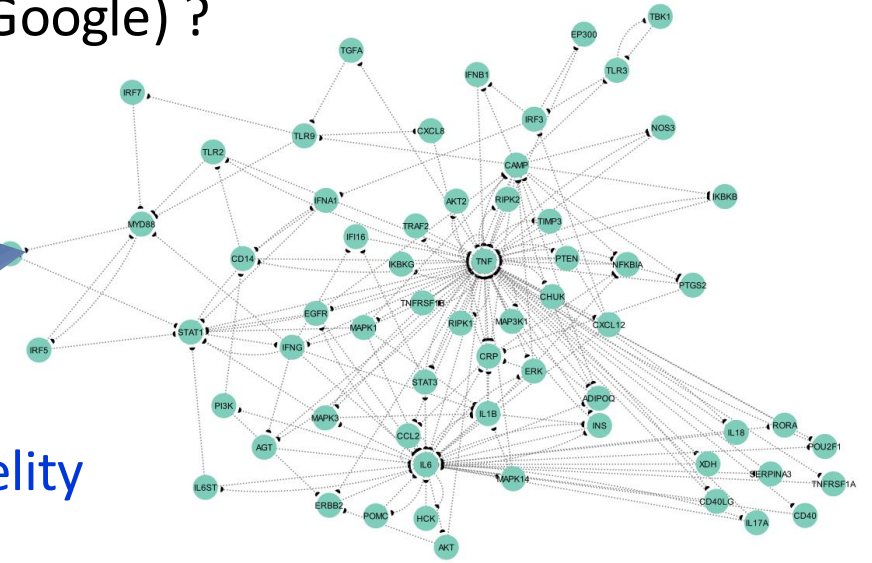
CPU chip



GPU chip



TPU (Google) ?



Increased fidelity

U Sask Copernicus HPC



GPU-accelerated modeling of biological regulatory networks

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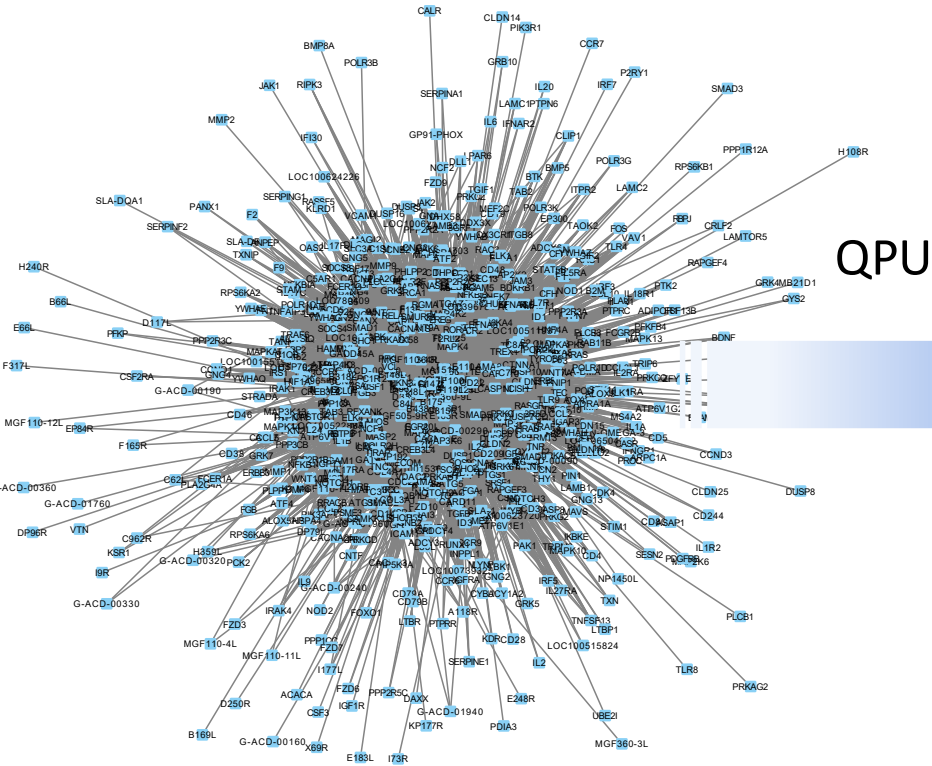
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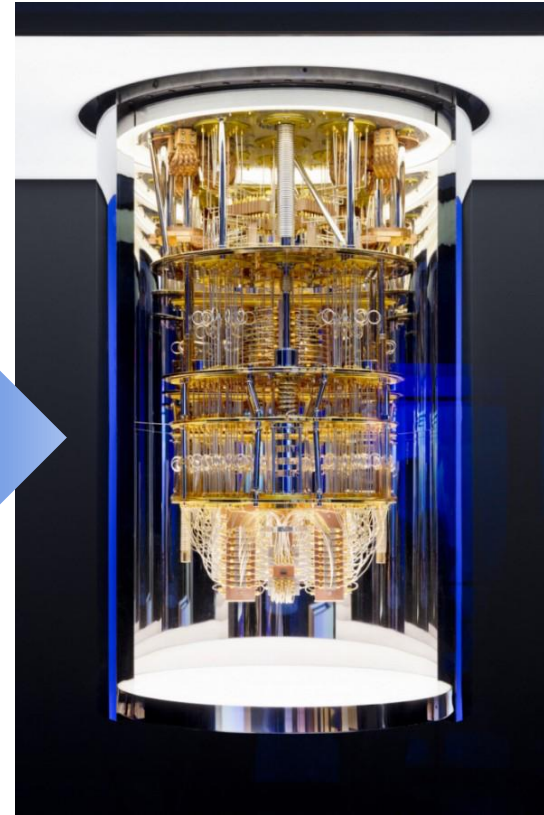
Pushing scale

Pathogen-host interactome



African Swine Fever Virus

~ 700 proteins linked by ~9000 interactions



IBM Quantum System Two

'Heron' processor 133 superconducting qubits

quanTA  UNIVERSITY OF SASKATCHEWAN

IBM Quantum  PINQ²
PLATEFORME D'INNOVATION
NUMÉRIQUE ET QUANTIQUE

IEEE QCE 2025

Identifying Protein Co-regulatory Network Logic by Solving B-SAT Problems through Gate-based Quantum Computing

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Cross-disciplinary and embedded

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Numerical optimization,
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Engineering Science
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Quantum ML circuit design



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NLP, ML, Gen-AI



Jason Broderick, U4
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Quantum optimization

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Mathematics, U Sask

AI Logical reasoning and memory generation

Luis Gonzalez Dominguez, U4 (with Rayan Lab)
Mathematical Physics, U Sask
Quantum ML antigen pattern recognition

Student Alumni

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Biochemistry, Microbiology and Immunology (BMI)

Kira Comfort, BSc (cw Wilson, Khatooni, Tikoo labs)
Biochemistry, Microbiology and Immunology (BMI)

Across disciplines, colleges and institutions

It takes a village



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Major Science Initiatives Fund



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