Towards self-learning agents in era of high-throughput omics

Presenter: Ameen Eetemadi

Principal Investigator: Prof. Ilias Tagkopoulos

I use Blue Waters to:

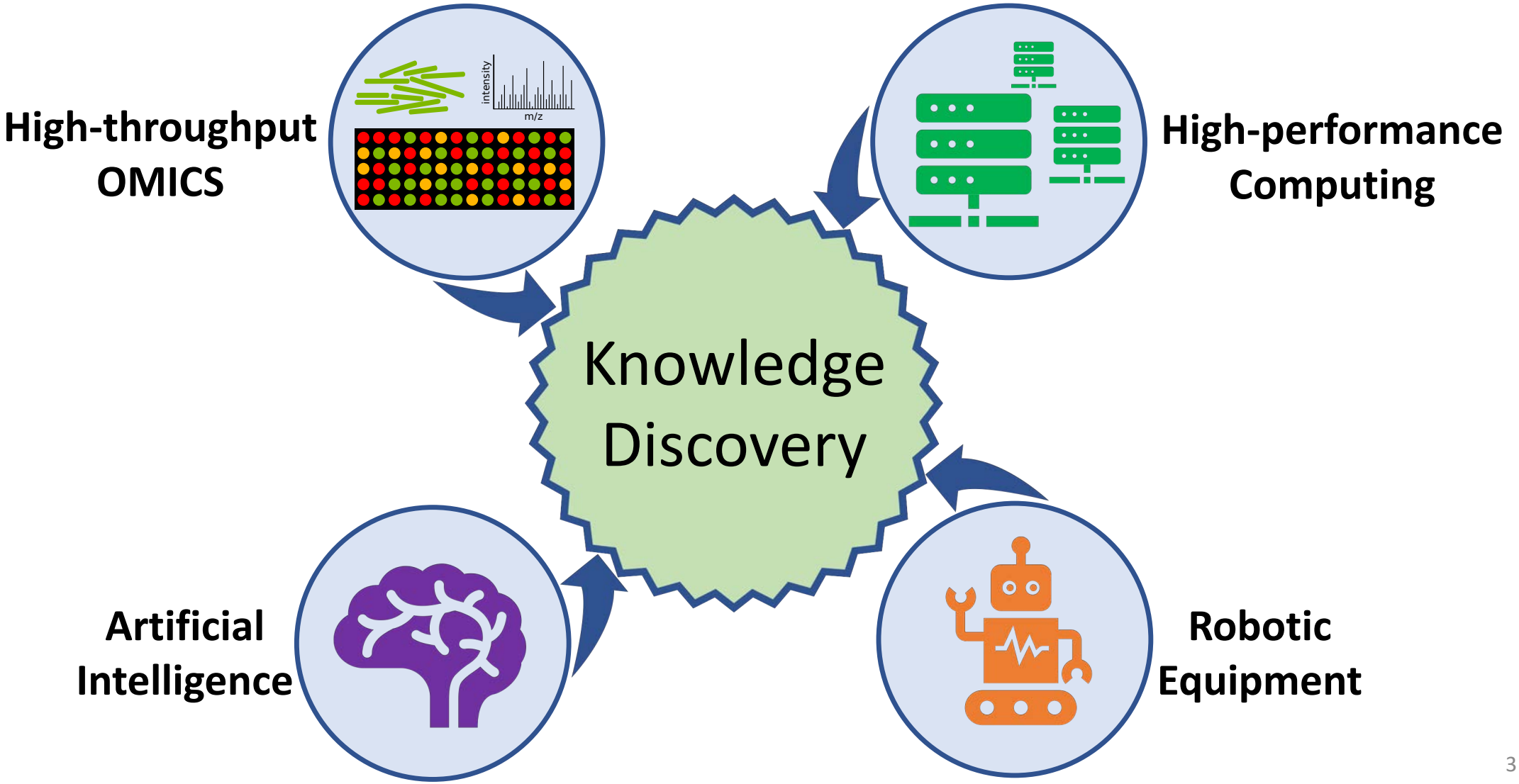
1. Design artificial neural networks for gene expression prediction

- Thermodynamic simulations
- Deep Learning
- Extensive evaluations

2. Determine optimal strategies to identify next set of experiments

- Synthetic data generation
- RNA-Seq data processing
- Gaussian Processes
- Extensive evaluations

We have entered a new era …



Goal: Efficient Knowledge Discovery

Maximize **knowledge** about *E. coli* Bacteria With Minimum **Cost**

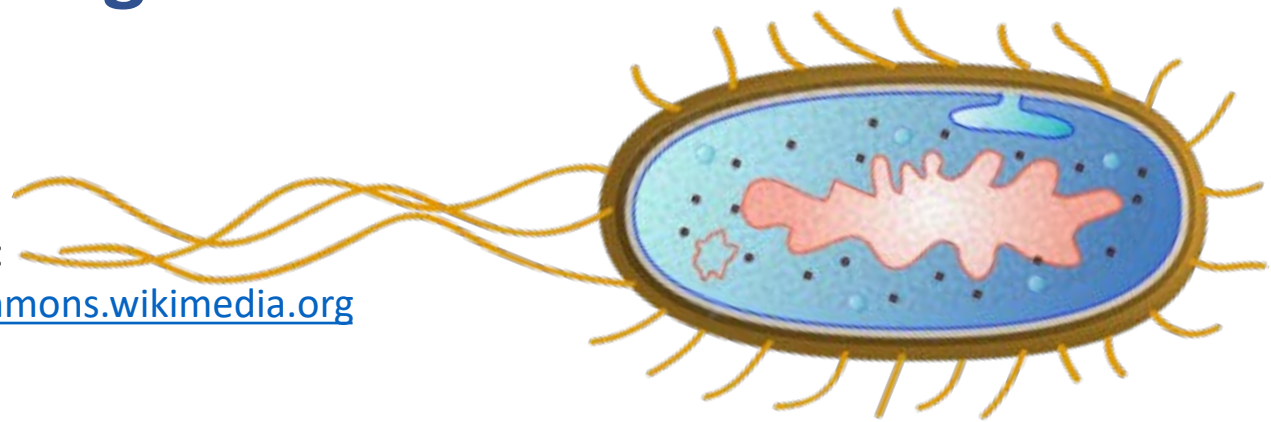


figure from:
https://commons.wikimedia.org

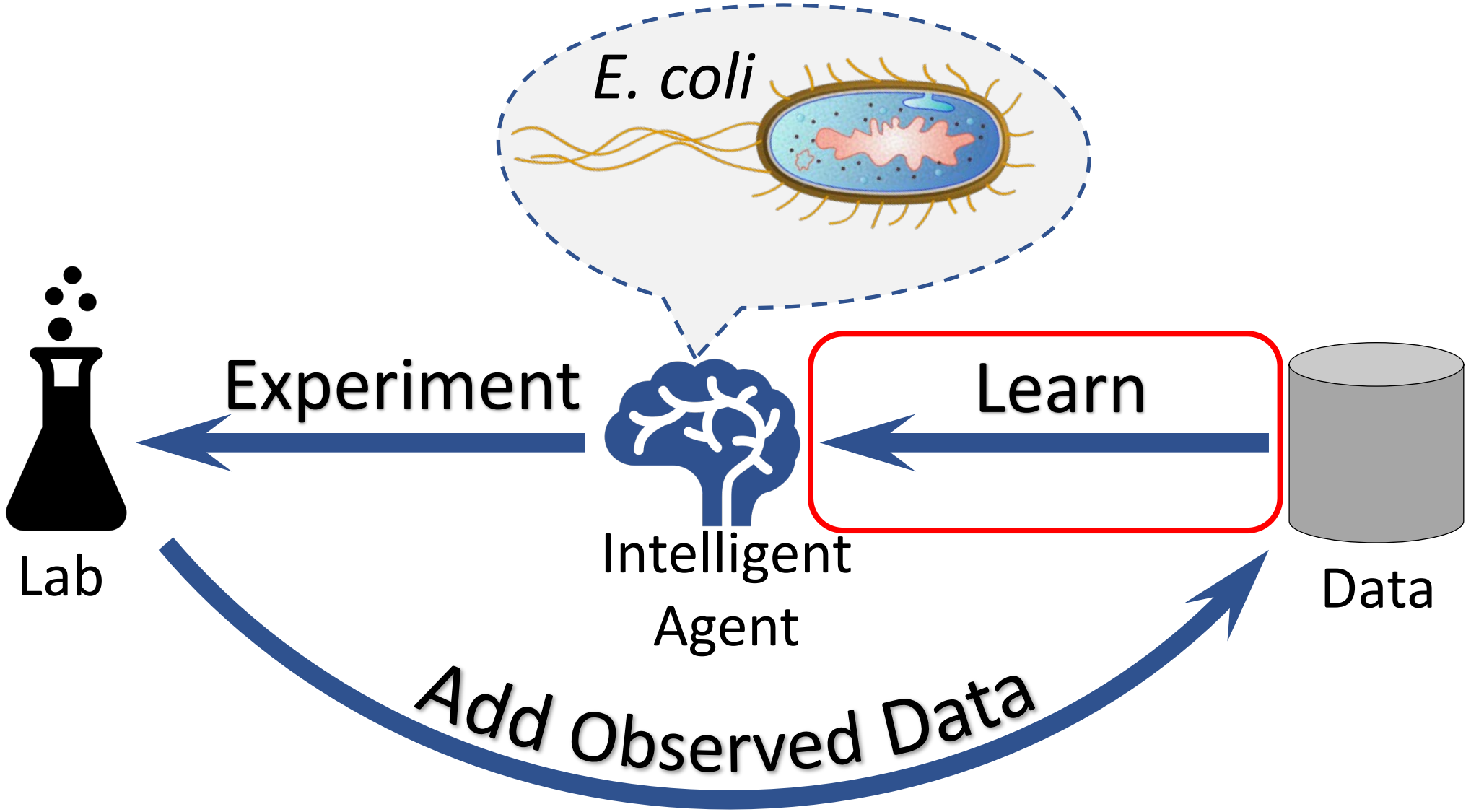
Applications

Medicine

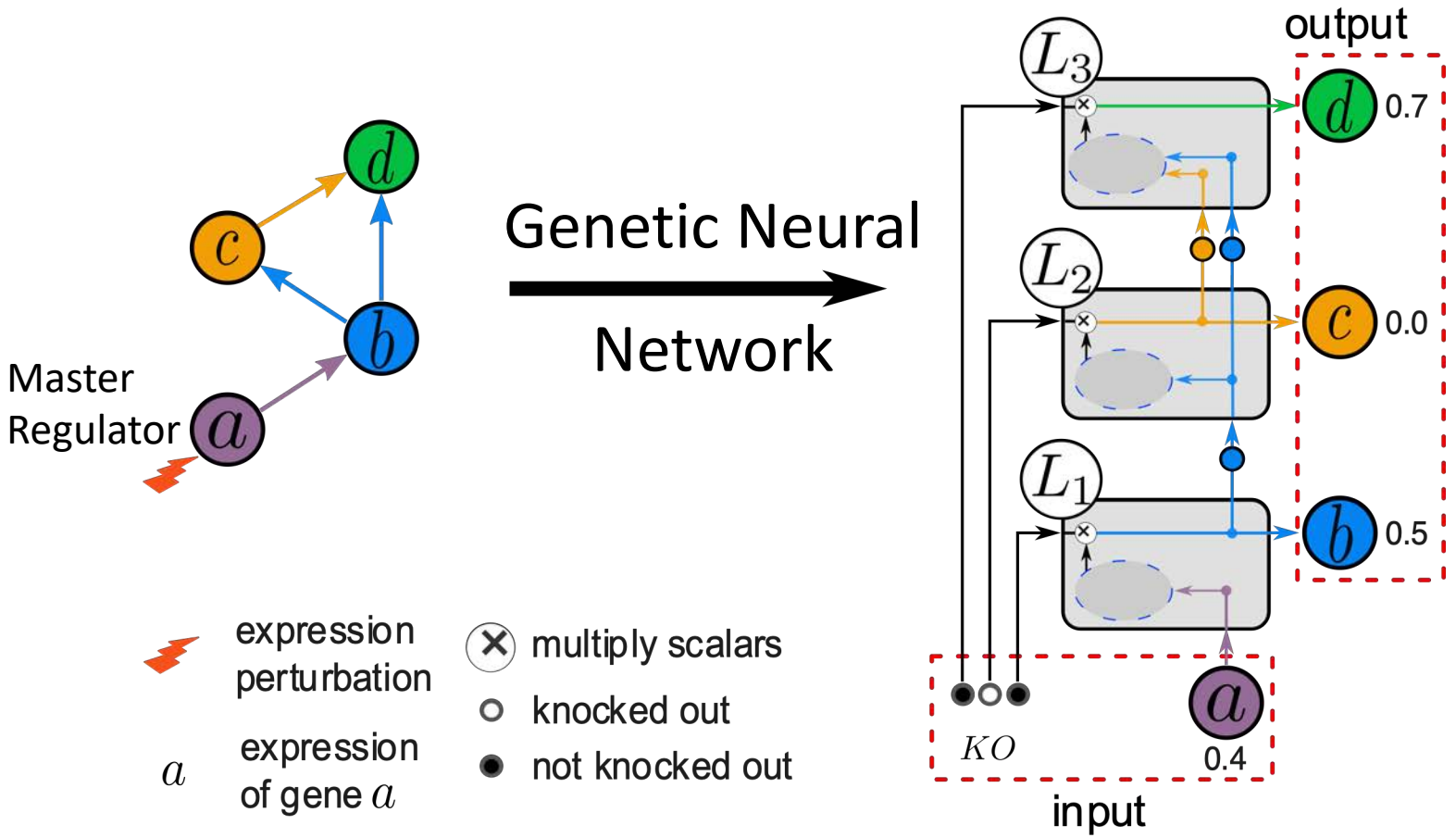
Food Safety

Basic Science

The Cycle of Knowledge Discovery



Learn dynamic program of a cell ⬇
Learn dynamics of gene expression in a cell

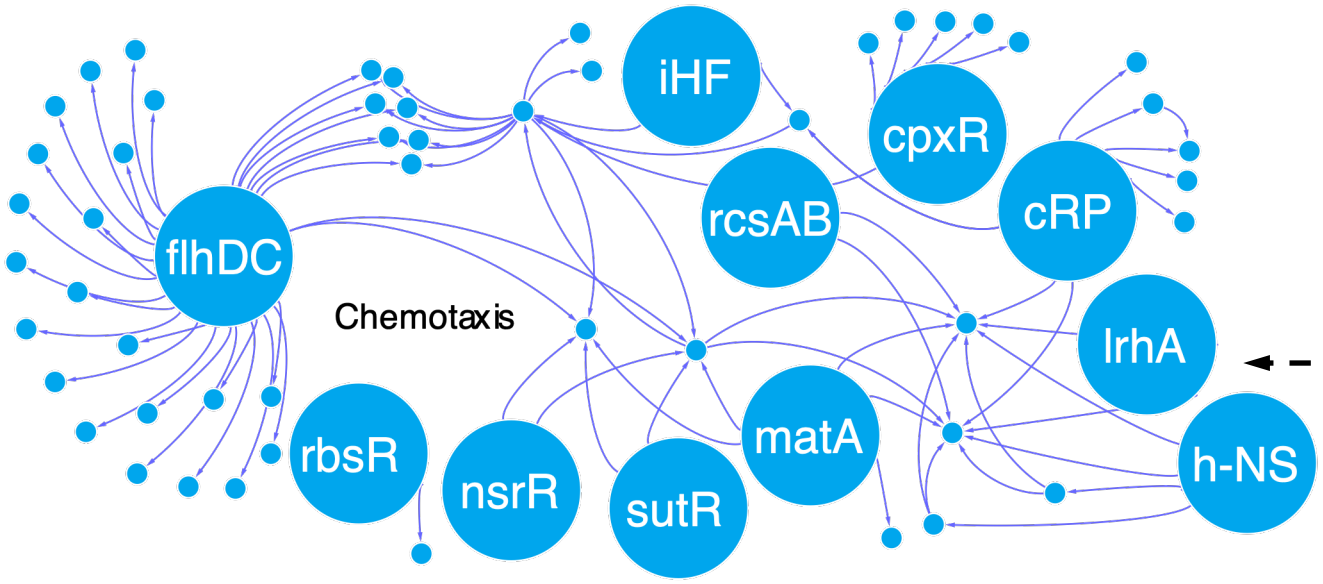


Key Features:

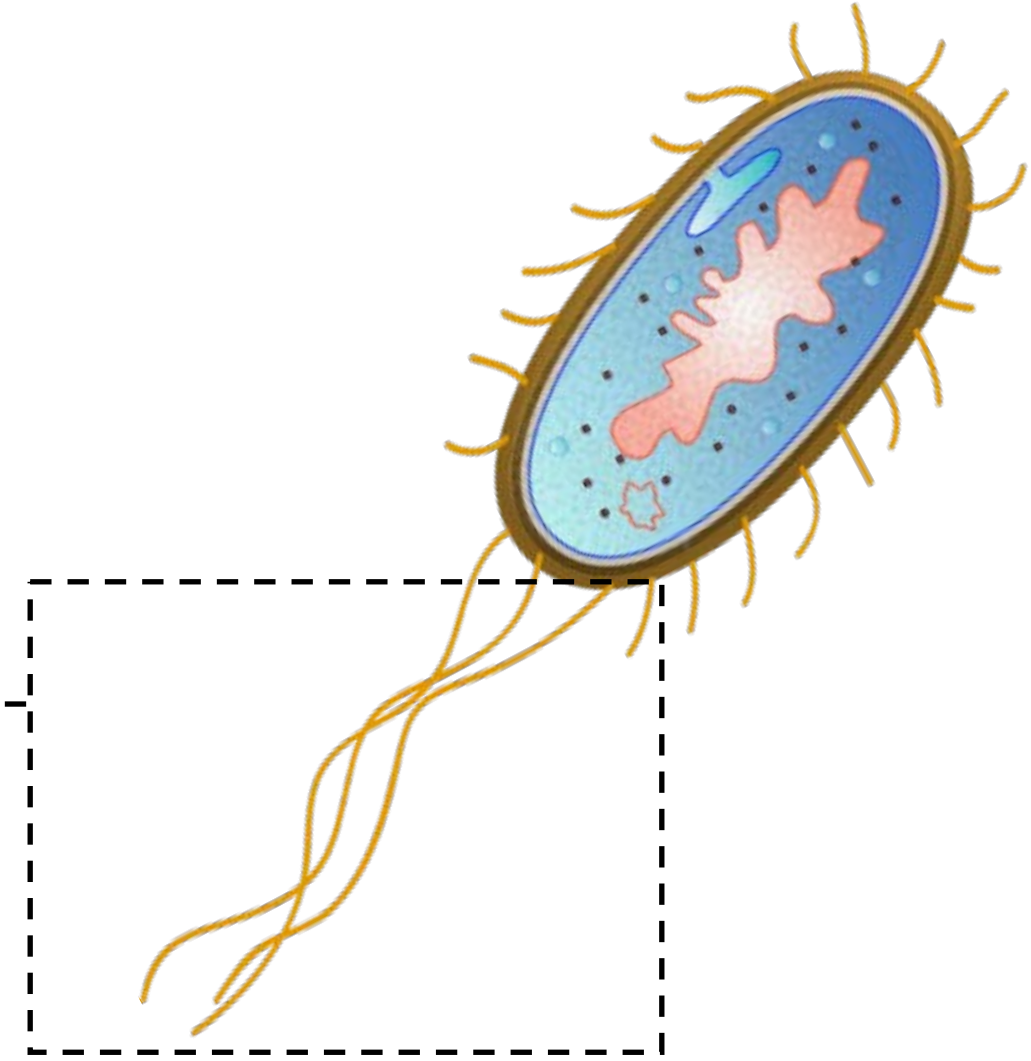
- Captures Regulatory Relationships
- Models Transcription Factor Dynamics

Published at:
Bioinformatics Journal, 2018

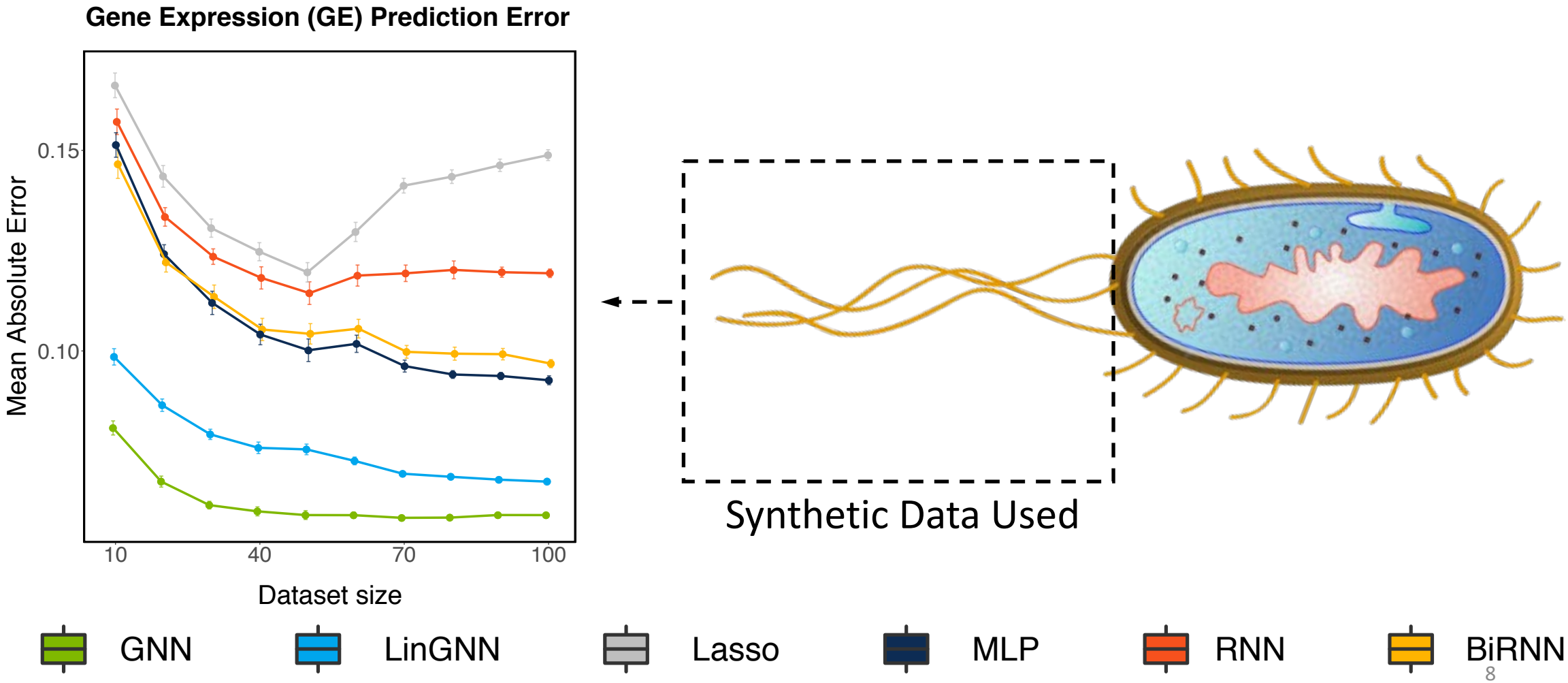
Learn dynamics of gene expression in *E. coli*



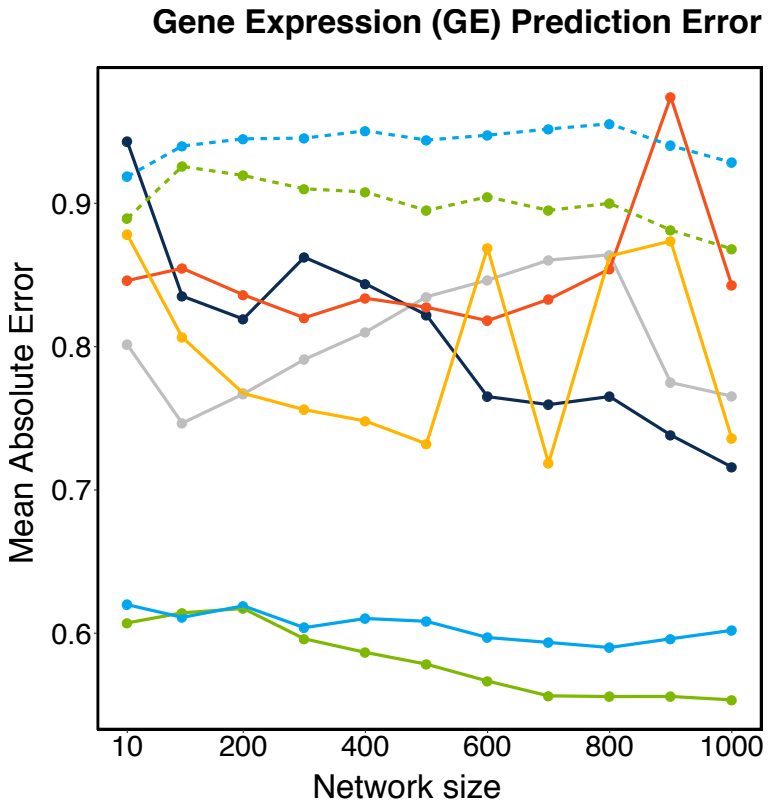
Chemotaxis Transcription Regulatory Network

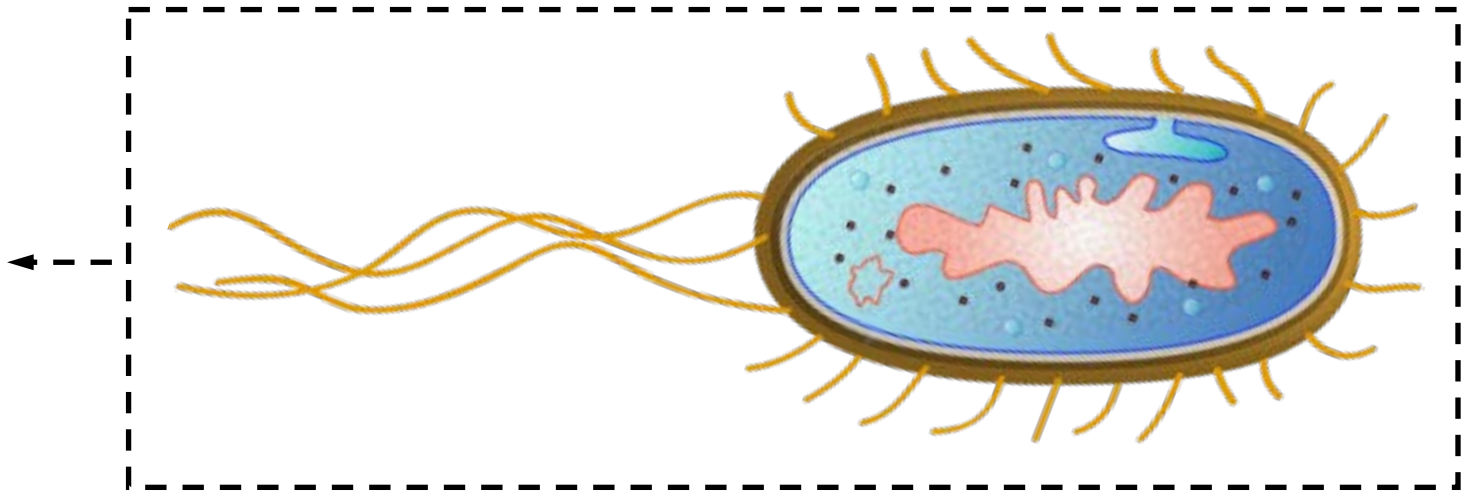


Genetic Neural Network (GNN) is 40% more accurate (for chemotaxis genes)



Genetic Neural Network (GNN) is 40% more accurate (for networks with 10-1000 genes)

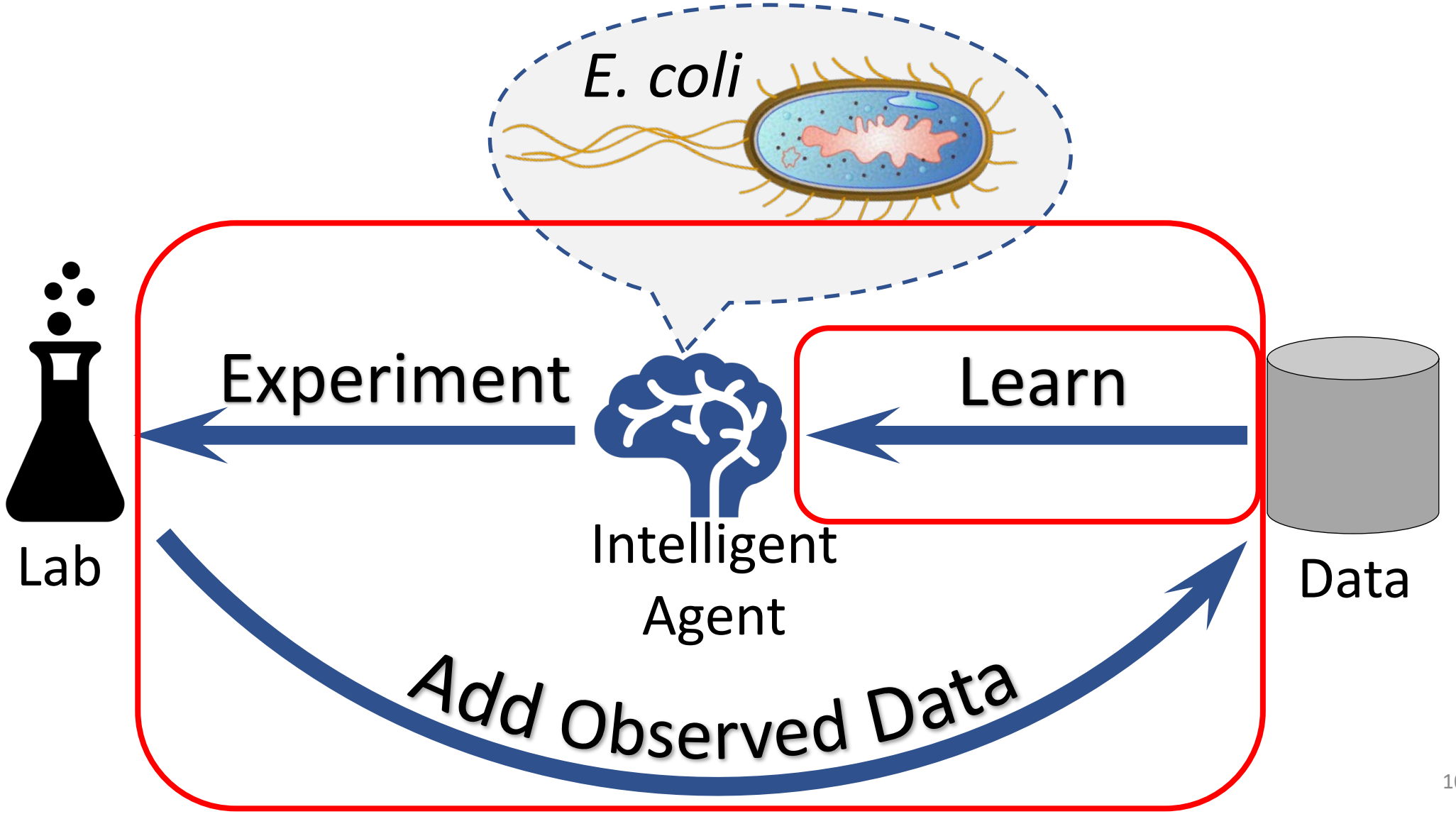




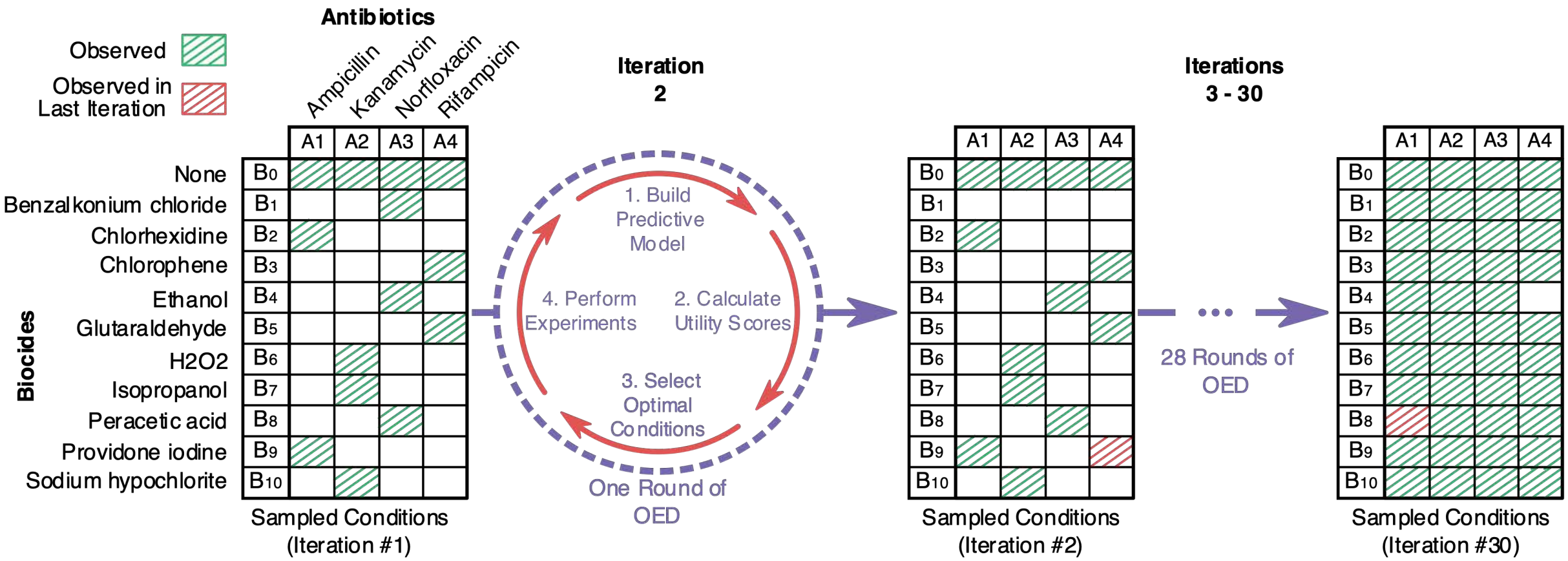
Real Data Used

GNN-rnd LinGNN-rnd GNN LinGNN Lasso MLP RNN BiRNN

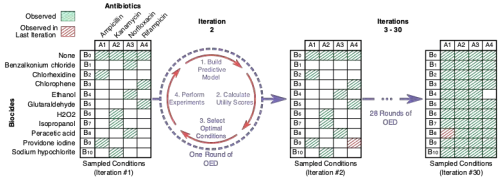
The Cycle of Knowledge Discovery



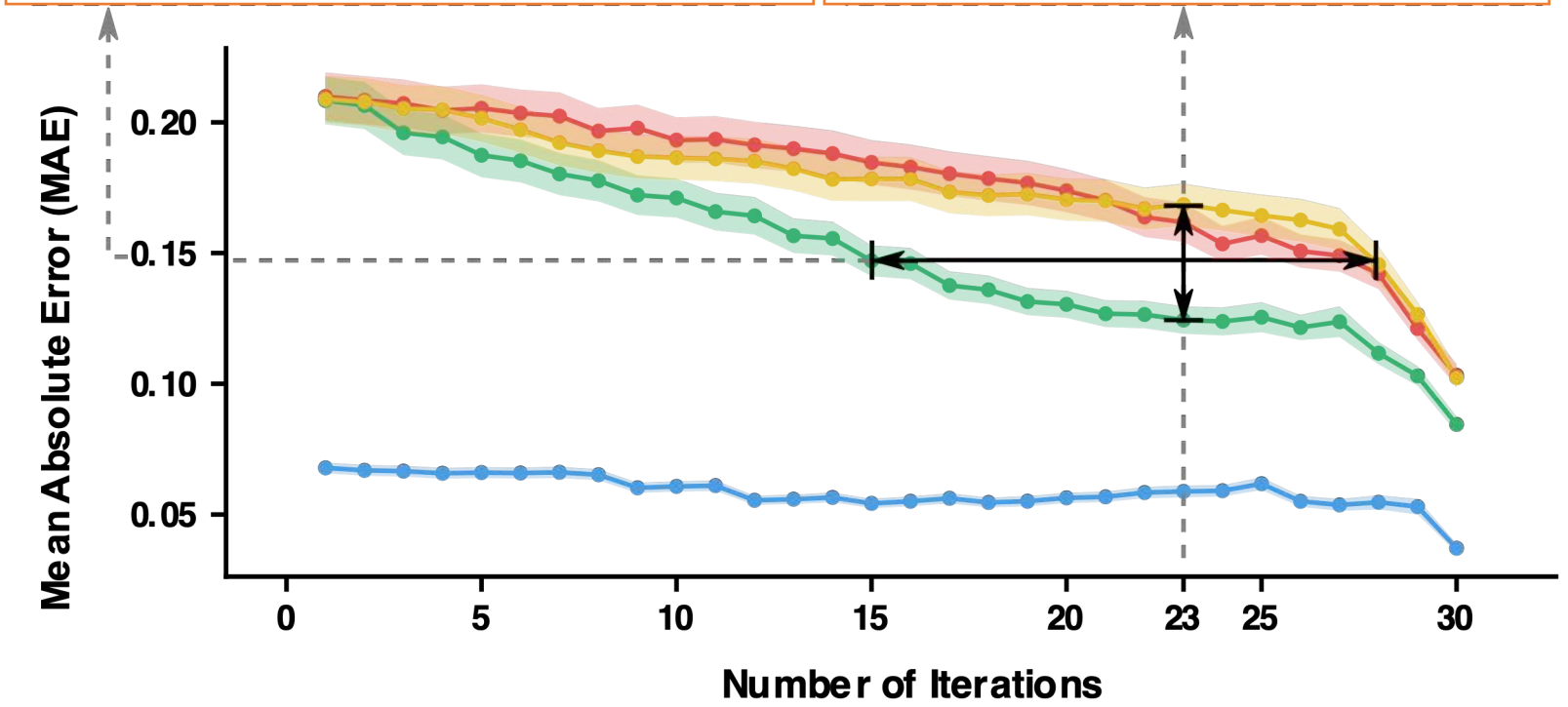
Optimal Experimental Design for Gene Expression Prediction



Accelerated Knowledge Discovery



Average Gene Expression Prediction Errors



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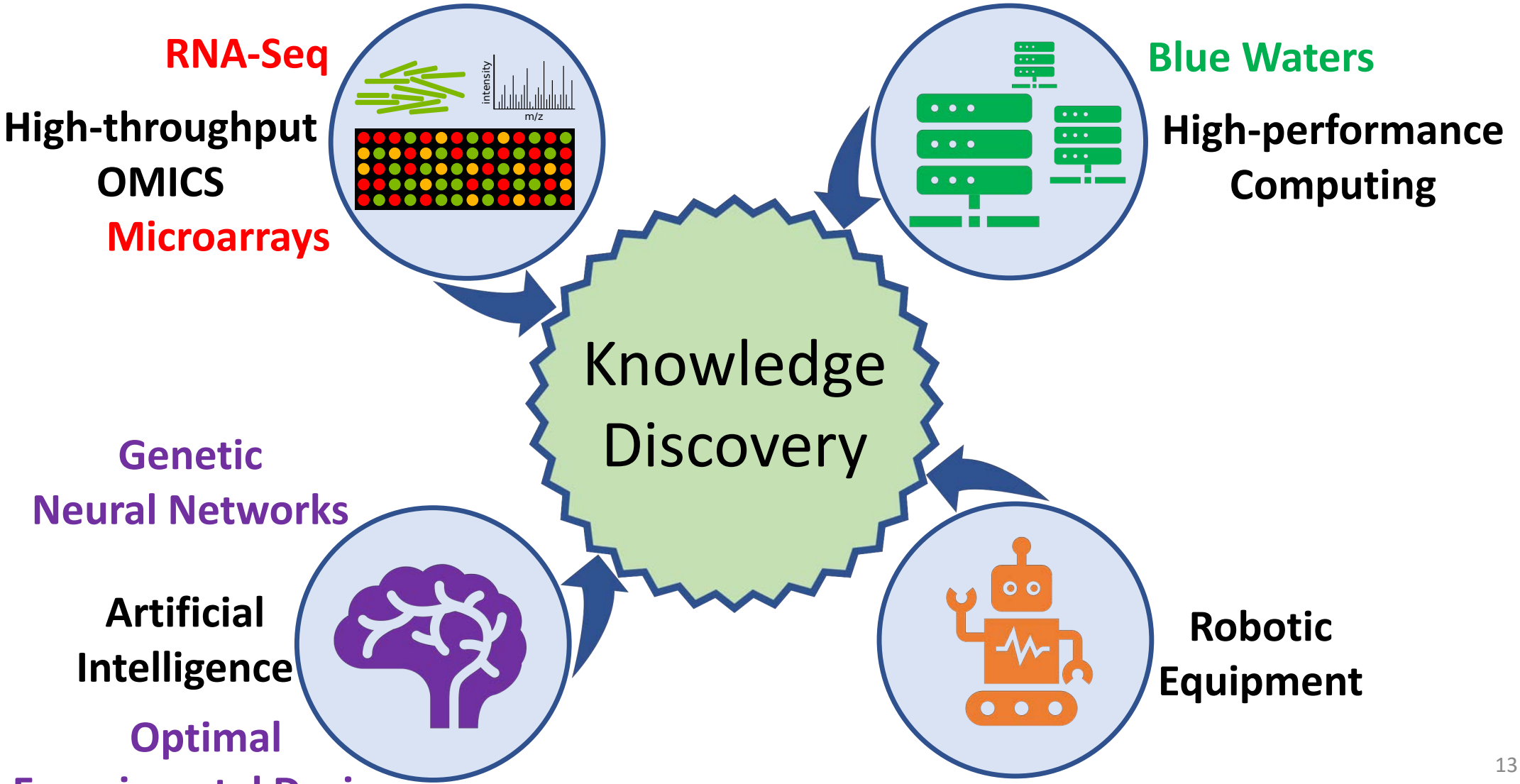

Blue Water Experience

Our Workload:

- Extremely parallel
- Independent small jobs

Advantages:

- Extremely reliable
- High availability
- Comprehensive documentation

BW Customer Support:

- Fast response
- High quality

Thank You!

Acknowledgements

- Ilias Tagkopoulos, PhD (Principal Investigator)
- Xiaokang Wang, PhD Candidate
- Navneet Rai, PhD
- Beatriz Merchel Piovesan Pereira, PhD Candidate

UC DAVIS
UNIVERSITY OF CALIFORNIA

Funding:

NSF