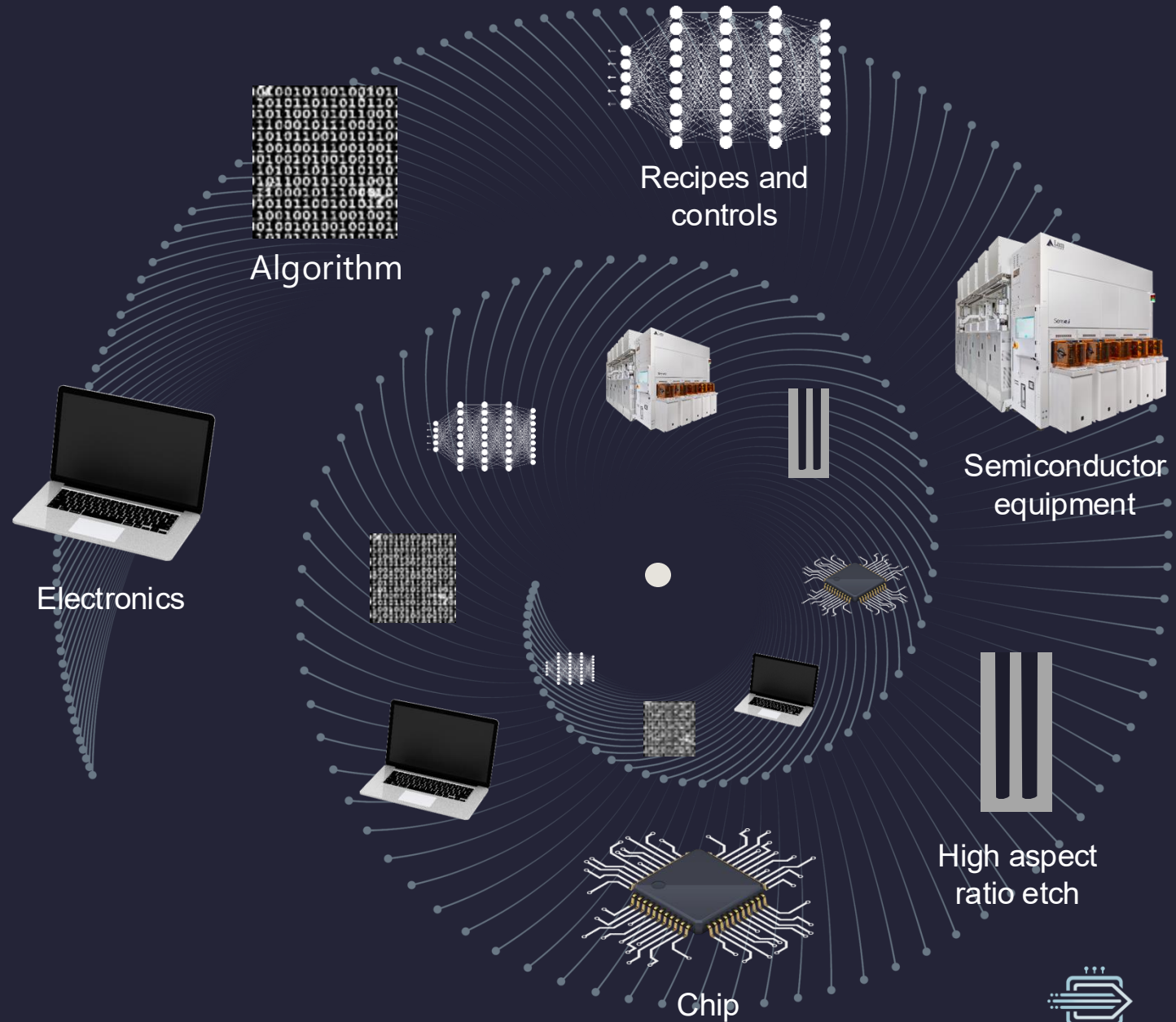
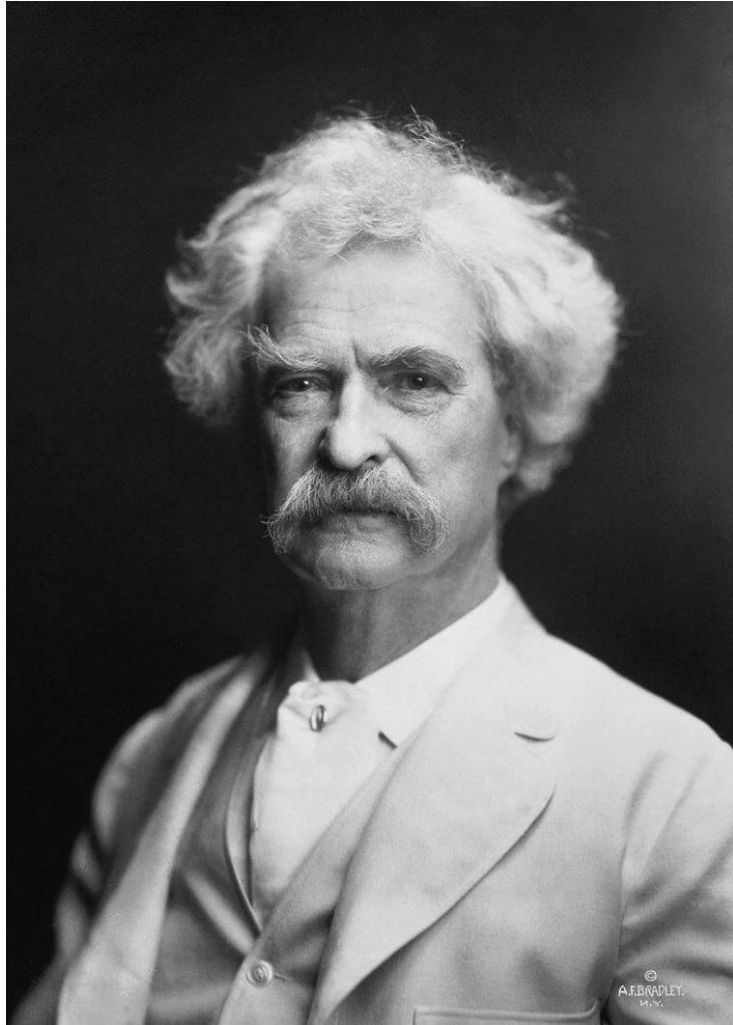


What goes around comes around: Using AI to make AI

Richard A. Gottscho, Ph.D.

President, SemiSan LLC
Former Exec VP and CTO of Lam Research

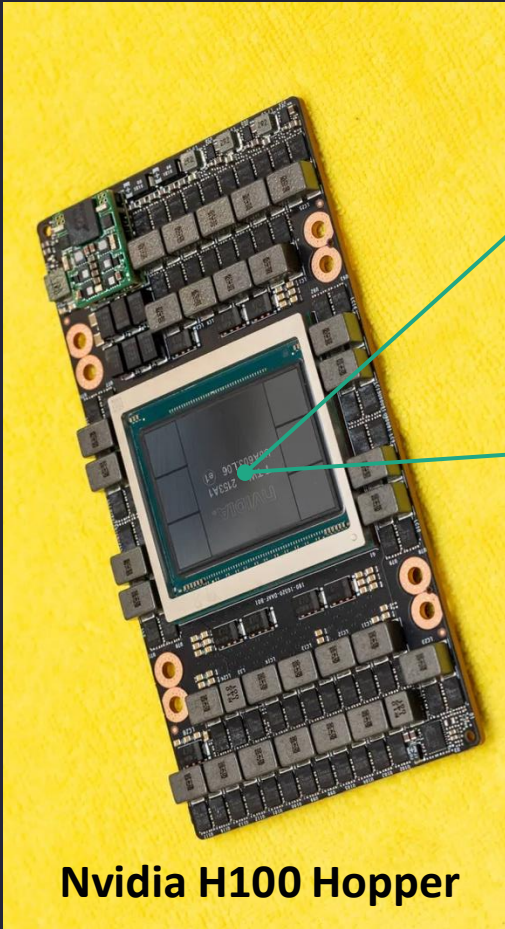




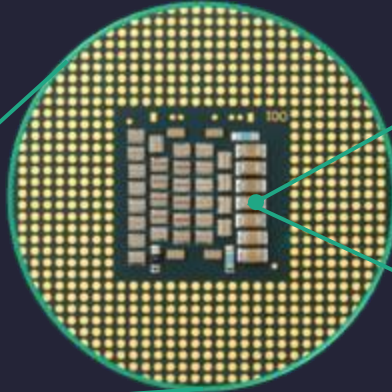
Mark Twain 1835-1910
American writer and humorist

It ain't what you don't know
that gets you into trouble.
It's what you know for sure
that just ain't so.

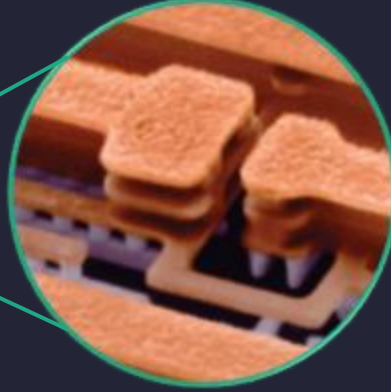
Inside every AI system are chips...



Nvidia H100 Hopper



At the heart of **every electronic product** is a complex microchip



Each chip contains billions of transistors that require advanced technologies to create



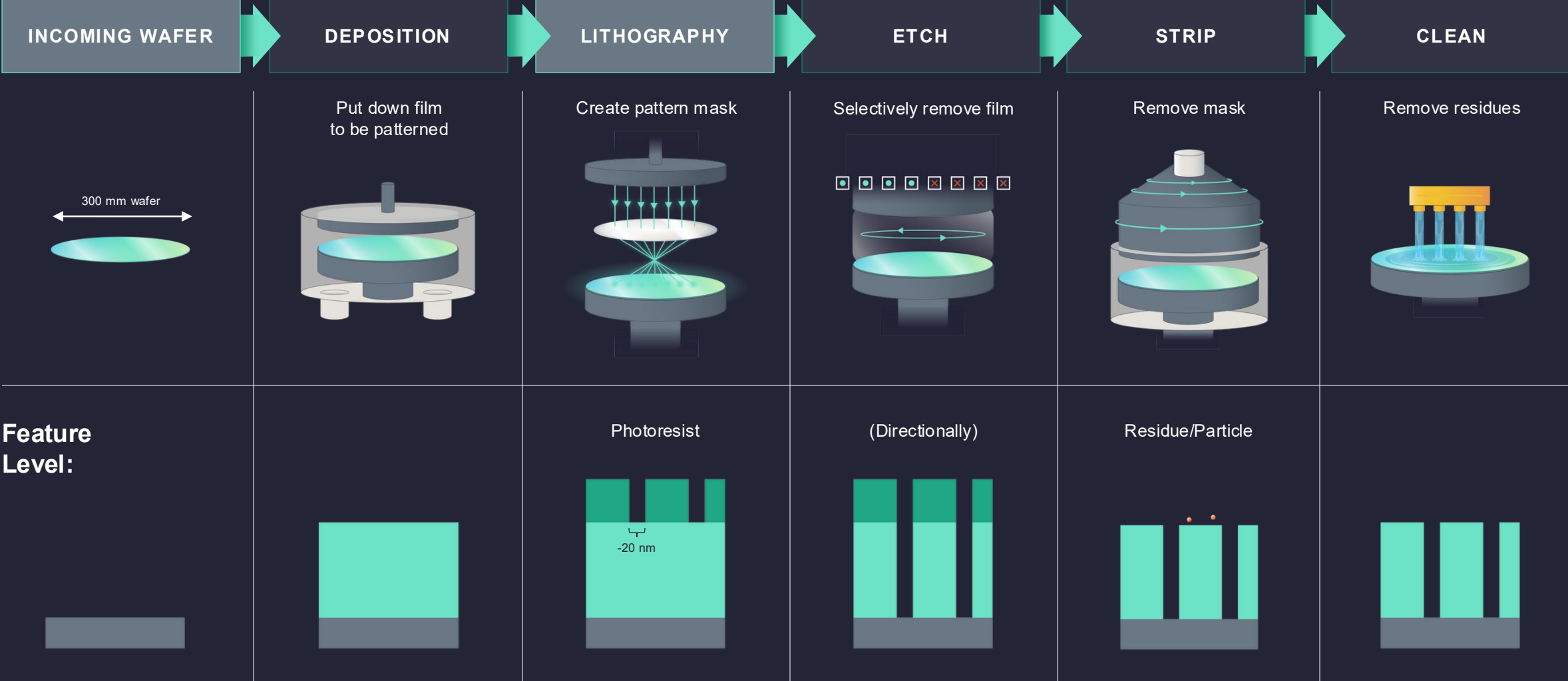
Lam's equipment is used to manufacture these semiconductor devices with as many as 1000 process steps



Innovative people, designing and developing the process

Lam wafer fabrication equipment is behind virtually every chip on the market.

How chips are made

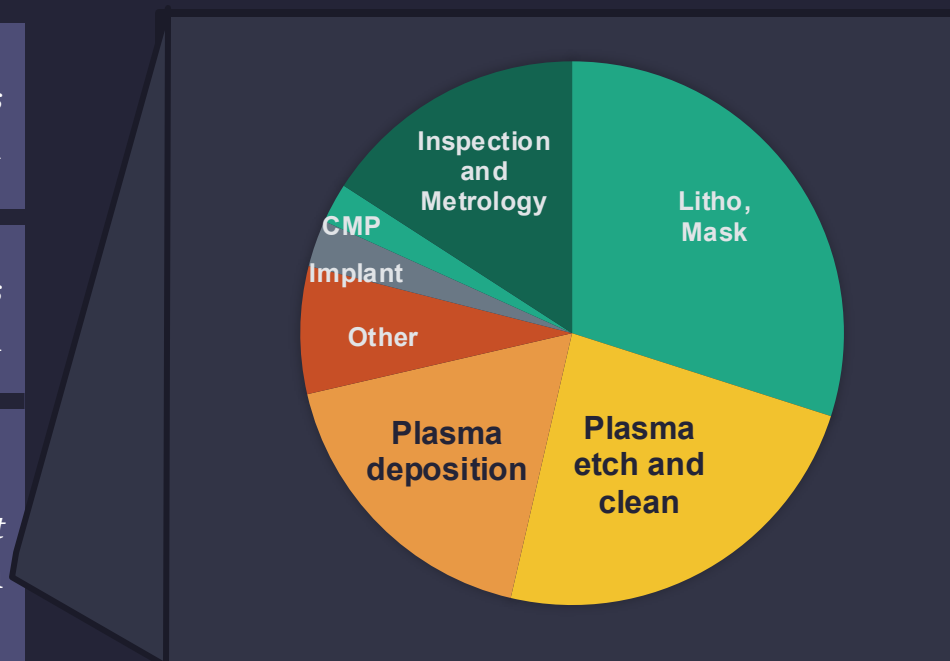


Wafer fab equipment enables semiconductor industry

2024



WFE segments

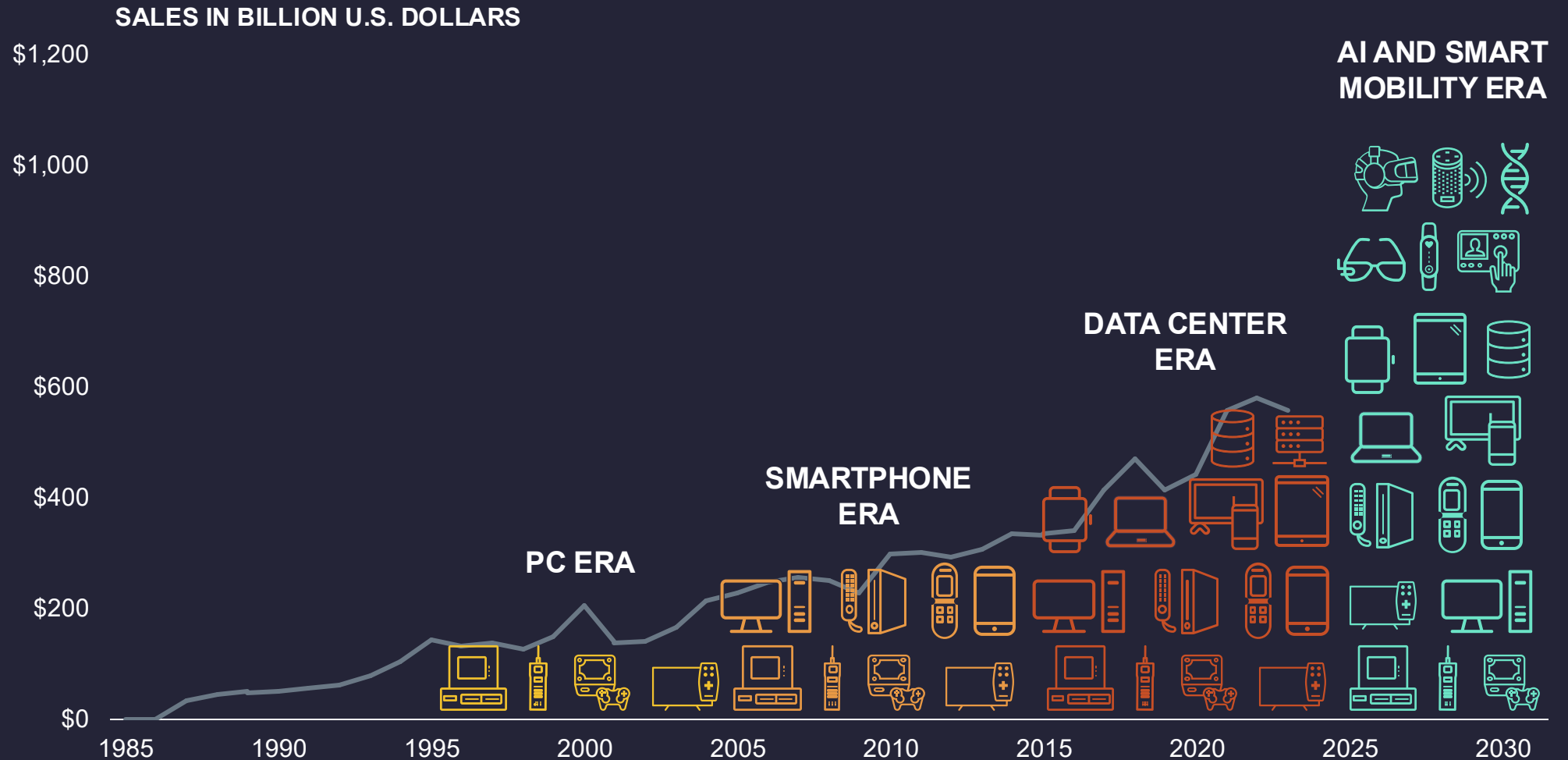


2024 WFE ranking

1	Applied Materials
2	ASML
3	Tokyo Electron
4	Lam Research
5	KLA

\$1 trillion semiconductor industry:

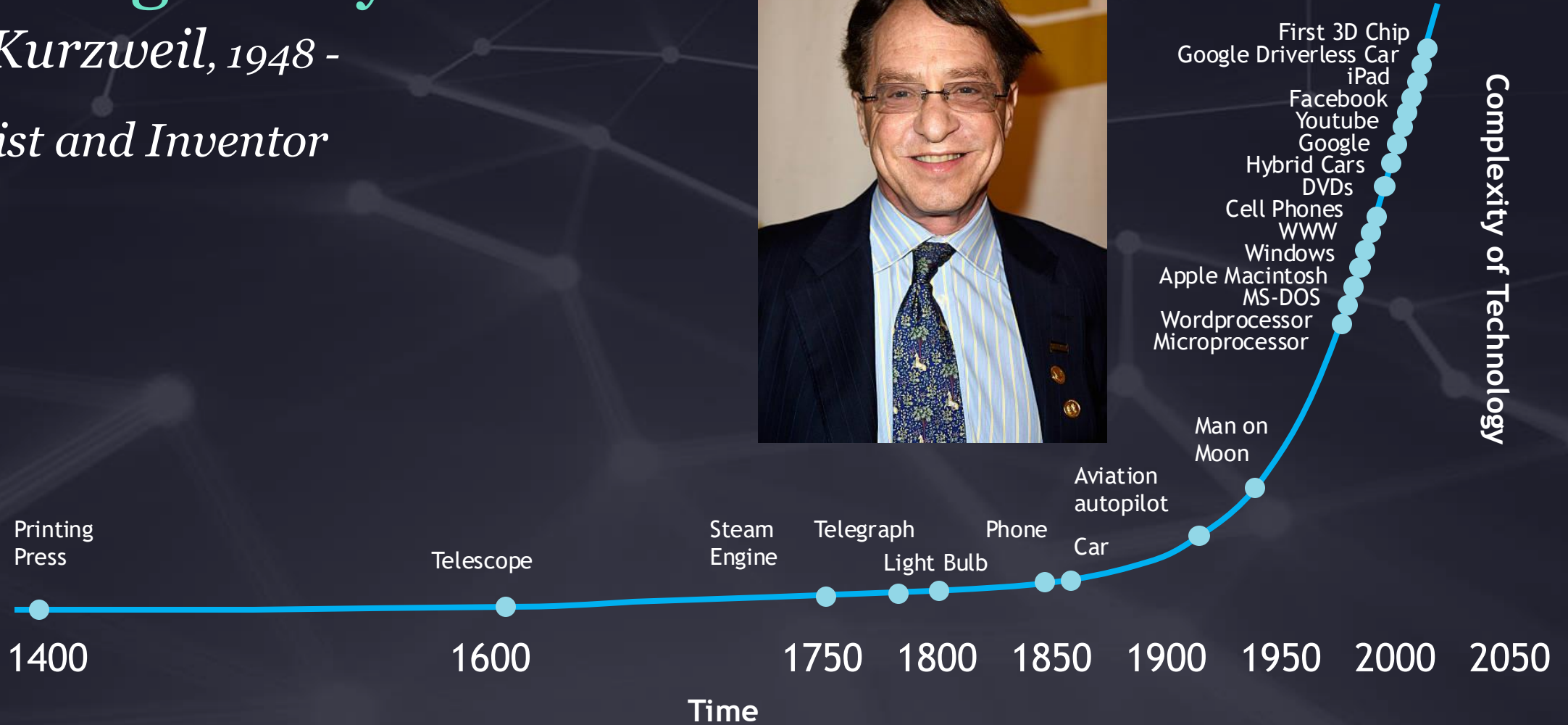
A multitude of drivers to amplify industry growth



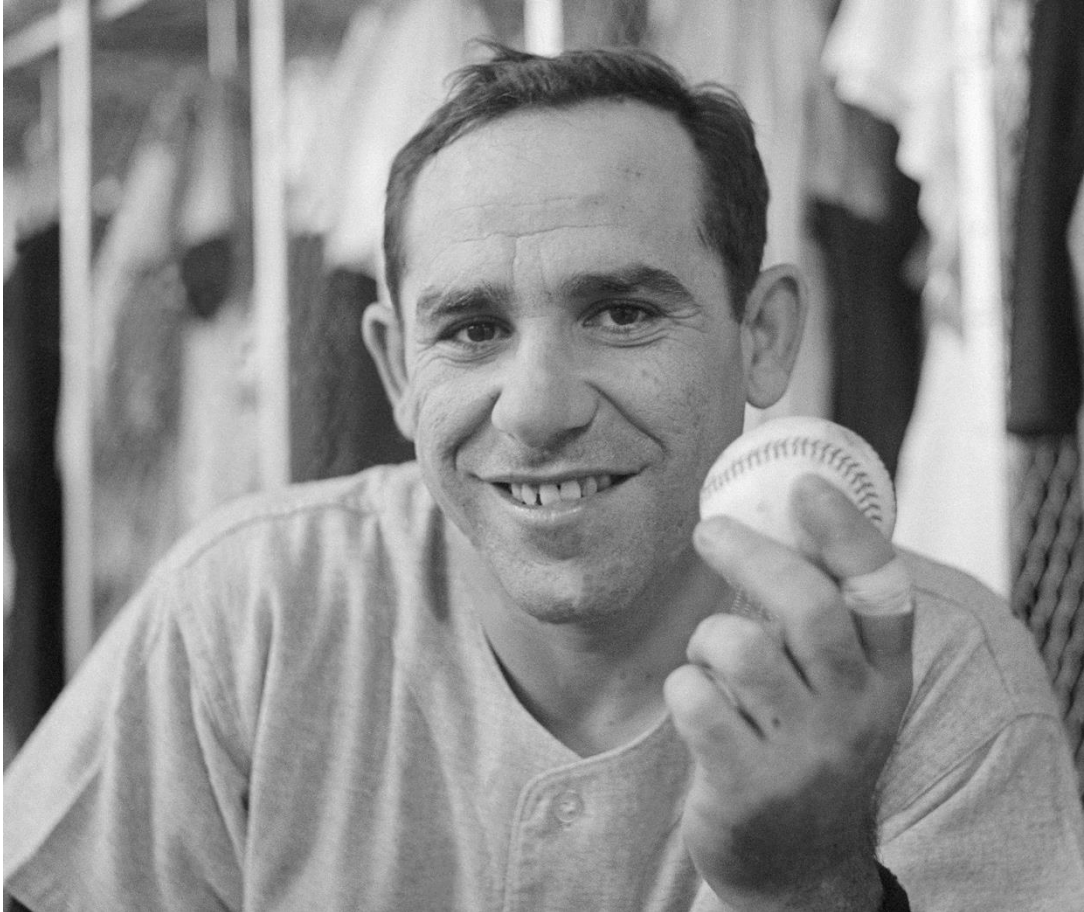
“The Singularity is Near”

Ray Kurzweil, 1948 -

Futurist and Inventor



“The future ain’t what it used to be”



Yogi Berra, 1925-2015
NY Yankee

The *Semiverse* is Lam's vision for a new digital ecosystem: a seamlessly integrated digital and physical network created to foster creativity and problem solving through unprecedented global collaboration.

Tim Archer, Lam President & CEO,
Accelerating through the Semiverse, imec
International Technology Forum, May 2022



Semiverse for *10,000x lower cost*

Virtualization *leverages* (not replaces!) investment in physical assets and real experiments

Virtual experimentation saves time, money, and resources (per recipe)

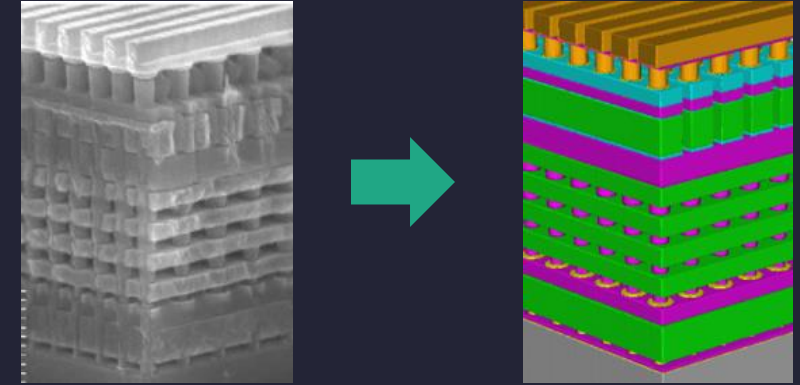
- Real experiments - \$1000, 0.5 days
- Simulated experiments - \$0.11, 8 mins
- Emulated simulations - \$3e-07, 0.0013 s

Virtual experimentation can be ubiquitous and an effective workforce training tool

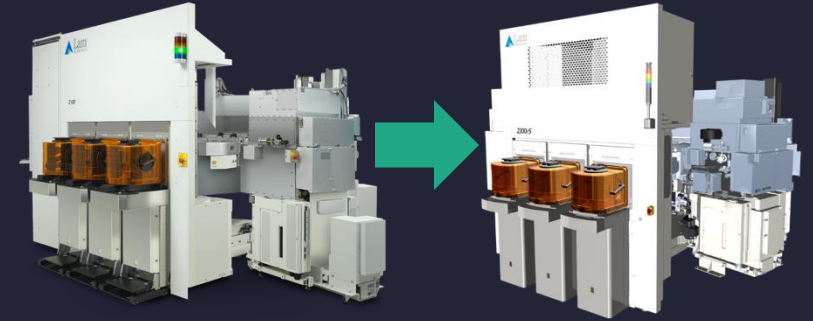
Barriers

- **Business model**
- **Some invention required**
- **Data sharing/ownership concerns**

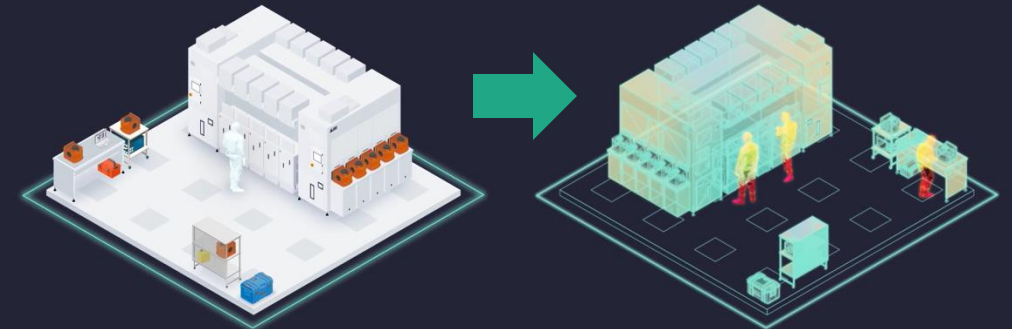
Virtual process:



Virtual tool:

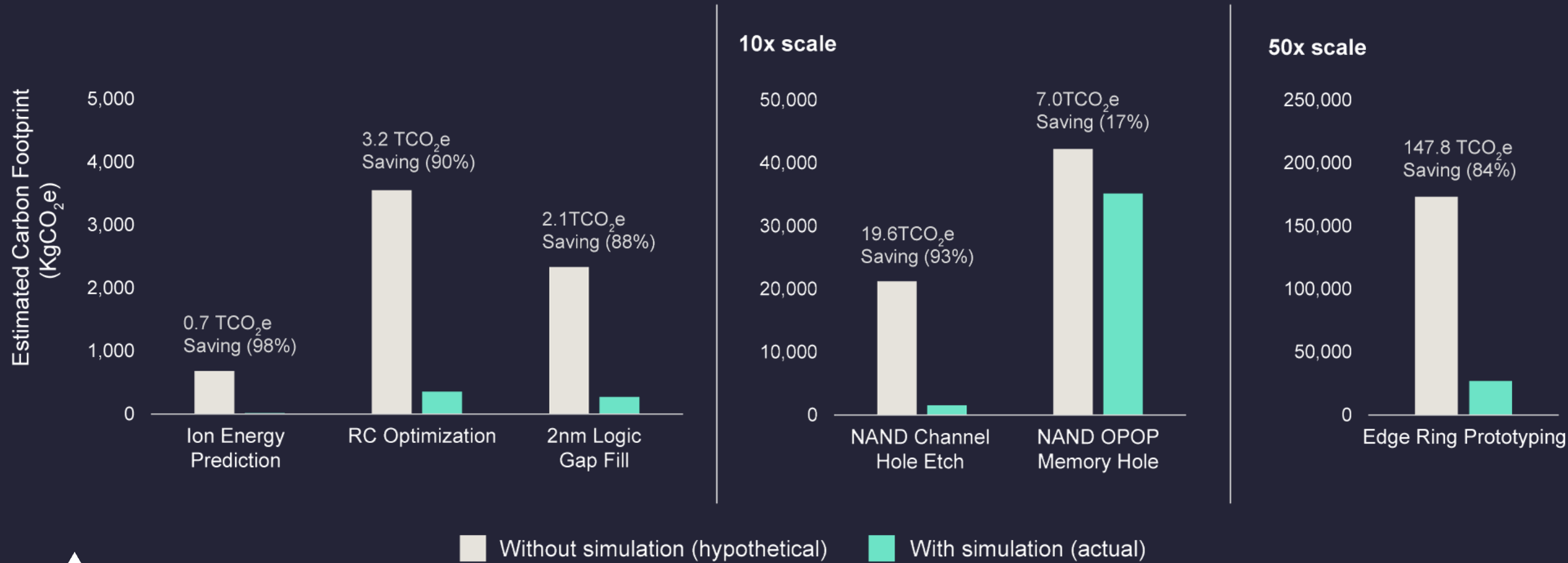


Virtual fab:



The Semiverse is GREENer

Every experiment investigated showed lower CO₂ equivalent from simulation



Reactor-scale twin

Simulate operating conditions in the chamber to predict and optimize process behaviors

The power of transformation



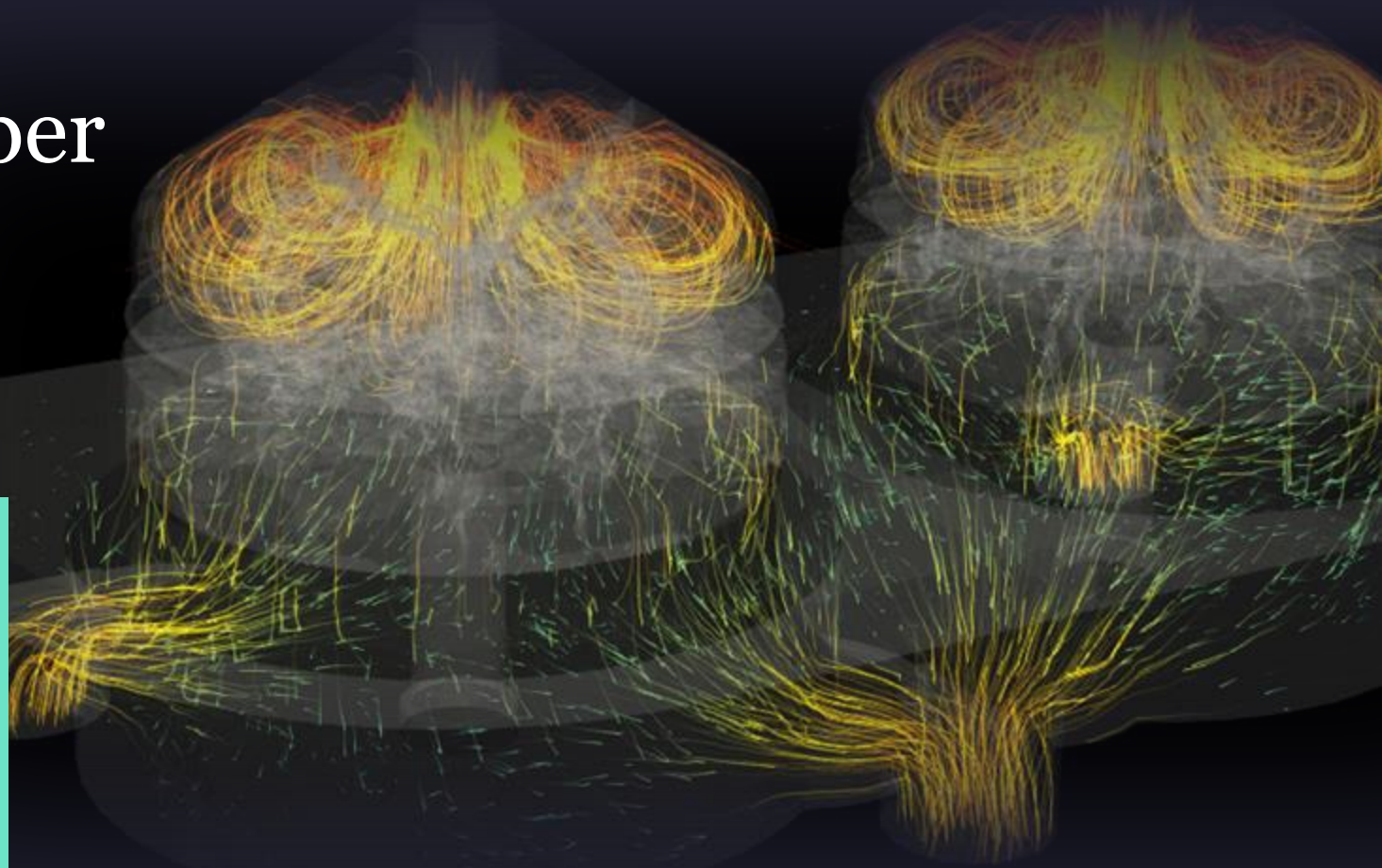
Reduce product development cycle time



Accurately estimate the etch or deposition rate on the entire wafer surface



Less waste with enhanced productivity



Equipment-scale twin

Improving first time right from design through install

The power of transformation



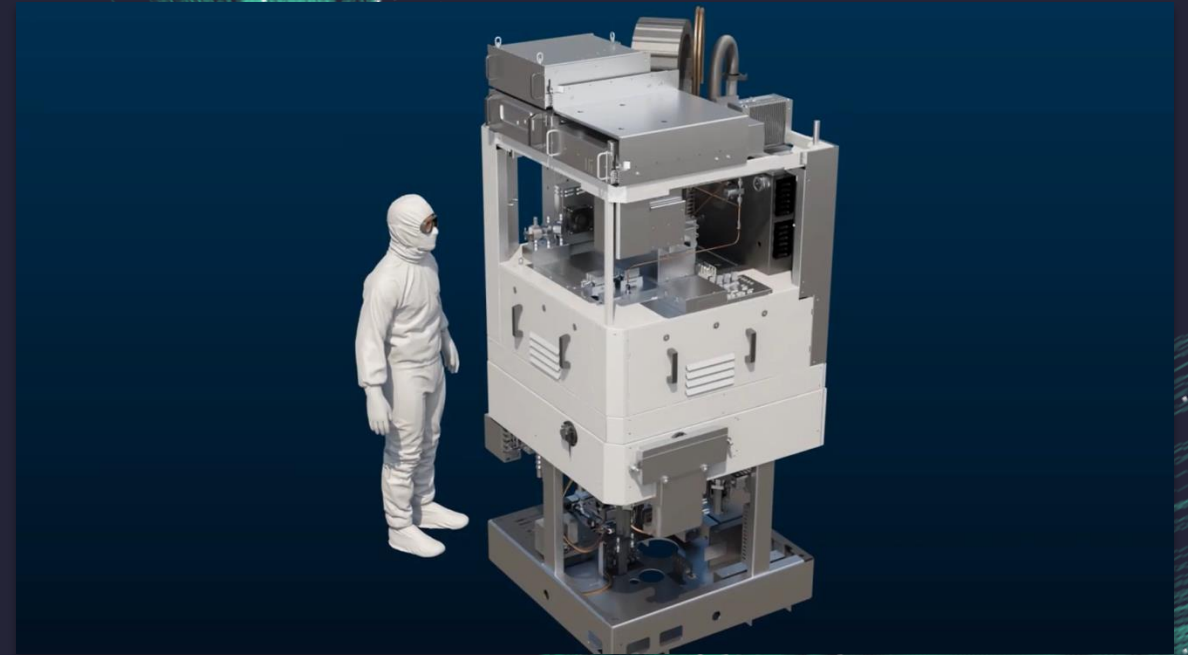
Virtual design, build, test, and verification
– find issues before physical build

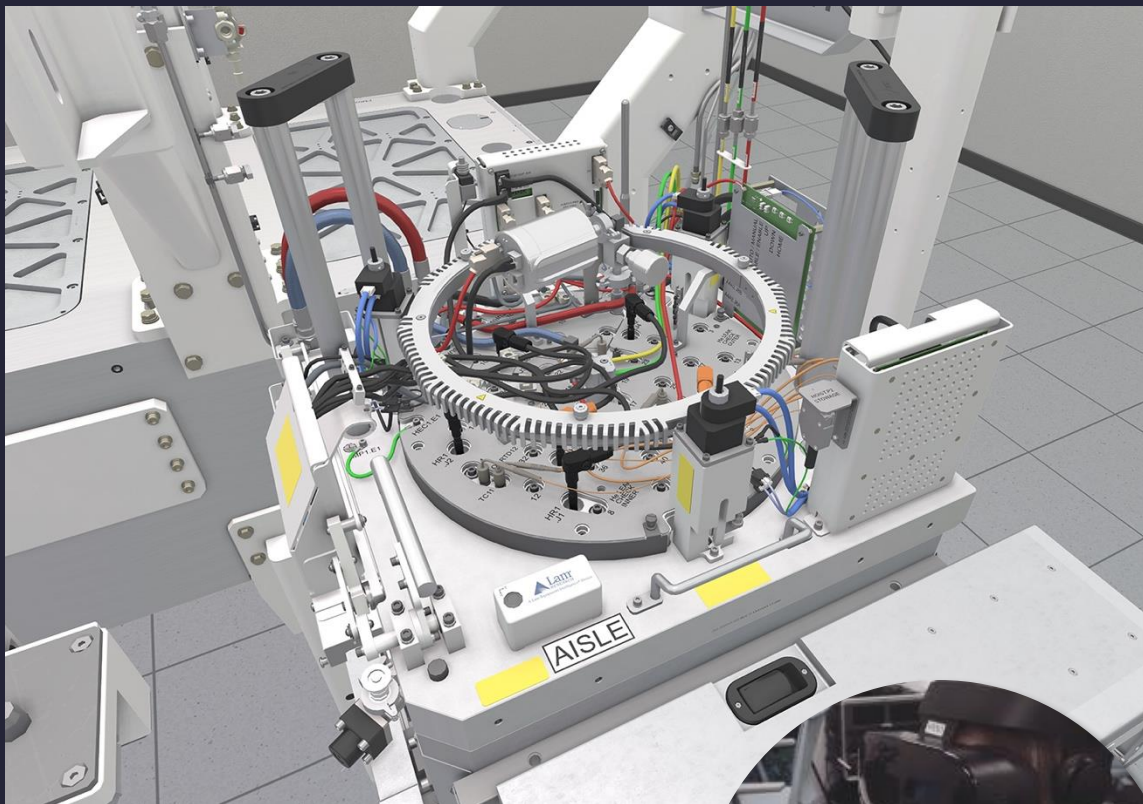


Design for manufacturing and serviceability



Less waste from fewer hardware iterations





Equipment-scale twin

Building equipment expertise faster and more effectively

The power of transformation

- ⊕ Provides faster more complete learning for engineering workforce
- ⊕ Allows more frequent refresher training and content updates
- ⊕ Enable earlier access to new product training

Equipment-scale twin

Reducing tool downtime with AI and AR enabled troubleshooting



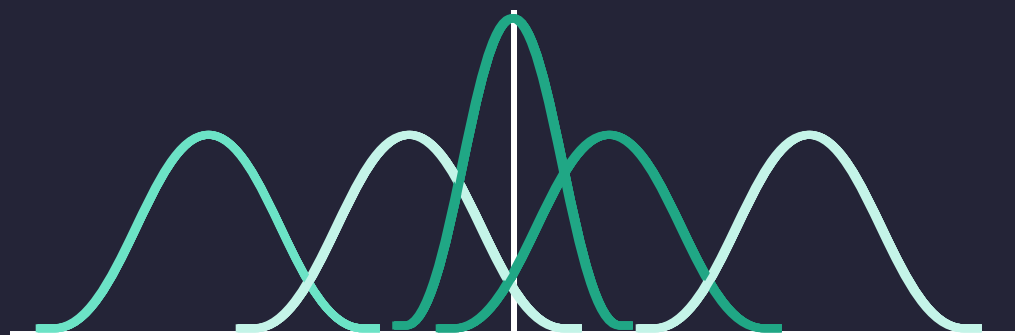
The power of transformation



AI identifies problem and prescribes fix using data and learning from various sources



Minimizes engineering service labor and cost



Fab-scale twins

Using machine learning to achieve yield faster with chamber matching and fleet optimization

The power of transformation

- ⊕ Accelerate chamber matching during install, shortening time to tool qualification
- ⊕ Minimizes fleet performance variability
- ⊕ Reduces engineering service labor



Semiconductor Manufacturing and Advanced Research with Twins

<https://www.smartusatwins.org/>

Digital Twins for Smarter Semiconductor Manufacturing



Ask ChatGPT

Please provide a summary of the state-of-the-art in the use of machine learning to optimize semiconductor chip manufacturing

Thought for 13 seconds...

Machine learning (ML) has rapidly been **adopted across semiconductor manufacturing**, transitioning from traditional rule-based control to data-driven, adaptive systems. State-of-the-art ML methods now permeate every facet of semiconductor chip manufacturing—from **virtual metrology** and **yield enhancement** to **recipe tuning**, **scheduling**, and **design automation**.

Ongoing advancements in explainability, federated training, and quantum-inspired algorithms are poised to drive the next wave of efficiency, quality, and agility in semiconductor fabs.

References included in further reading list at end of this presentation

Some Pertinent References

- E.A Rietman and E.R. Lory, “Use of neural networks in modeling semiconductor manufacturing processes: an example for plasma etch modeling.” *Semiconductor Manufacturing, IEEE Transactions on Semiconductor Manufacturing* 6(4):343 – 347 (**1993**)
- Anirudh et al., "2022 Review of Data-Driven Plasma Science," *IEEE Trans. Plasma Sci.*, vol. 51, no. 7, July 2023.
Plasma science is entering a **transformative data-driven era**
Core technologies:
 Surrogate modeling & **Physics-Informed** Neural Networks (PINNs)
 Workflow automation, visualization, and **uncertainty** quantification
- Y.-L. Chen *et al.*, “Exploring Machine Learning for Semiconductor Process Optimization: A Systematic Review.” Jul. 16, 2024. doi: 10.36227/techrxiv.172114788.85190557/v1
Optimize semiconductor manufacturing
Literature survey identifying 58 publications
- A. D. Bonzanini, K. Shao, D. B. Graves, S. Hamaguchi, and A. Mesbah, “Foundations of machine learning for low-temperature plasmas: **methods and case studies**,” *Plasma Sources Science and Technology*, vol. 32, no. 2, Feb. 2023, doi: 10.1088/1361-6595/acb28c.

Manufacturing leads the way with lots of cheap data

- For a typical fleet of tools
 - 100 sensors, 200 chambers
 - 2000 status variables
 - 100's of process steps
 - 5 Hz frequency
- How much data per fleet?
 - 5000 features extracted per wafer run
 - 100 million feature data points per day
 - 5-10 billion raw data points per day

AI in Chip Design

- **Automated Floor-planning & Placement**
 - Placing blocks (compute, memory, I/O) optimally.
 - Google's DeepMind-trained AI delivers better layouts for TPU chips in <24 hours
- **Generative EDA Tools**
 - ML models to explore countless design variants and optimize multi-objective trade-offs (power, timing, area).
 - Synopsys' DSO.ai applies ML to chip design workflows; Cadence's Cerebrus uses reinforcement learning for automatic optimization of placement, routing, and power use
- **Physics-aware & Antenna Modeling**
 - Co-design circuits with electromagnetic properties in mind.
 - Achieves faster and better designs for RF/wireless amplifiers—often beyond human capability



iln.ieee.org+12spectrum.ieee.org+12ece.engin.umich.edu+1

https://www.aegissofttech.com/insights/ai-in-semiconductor-industry/?utm_source=chatgpt.com

https://engineering.princeton.edu/news/2025/01/06/ai-slashes-cost-and-time-chip-design-not-all?utm_source=chatgpt.com

Why can't we design a process like we design a chip?

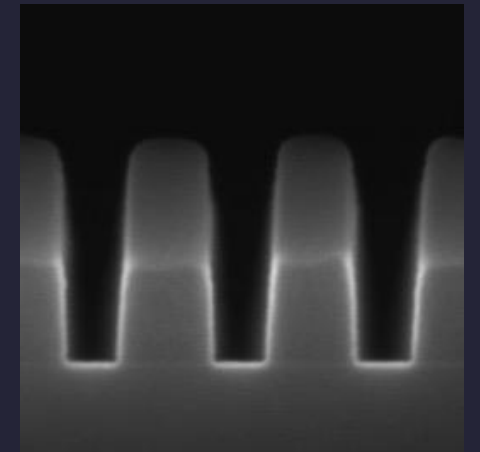
SPEC



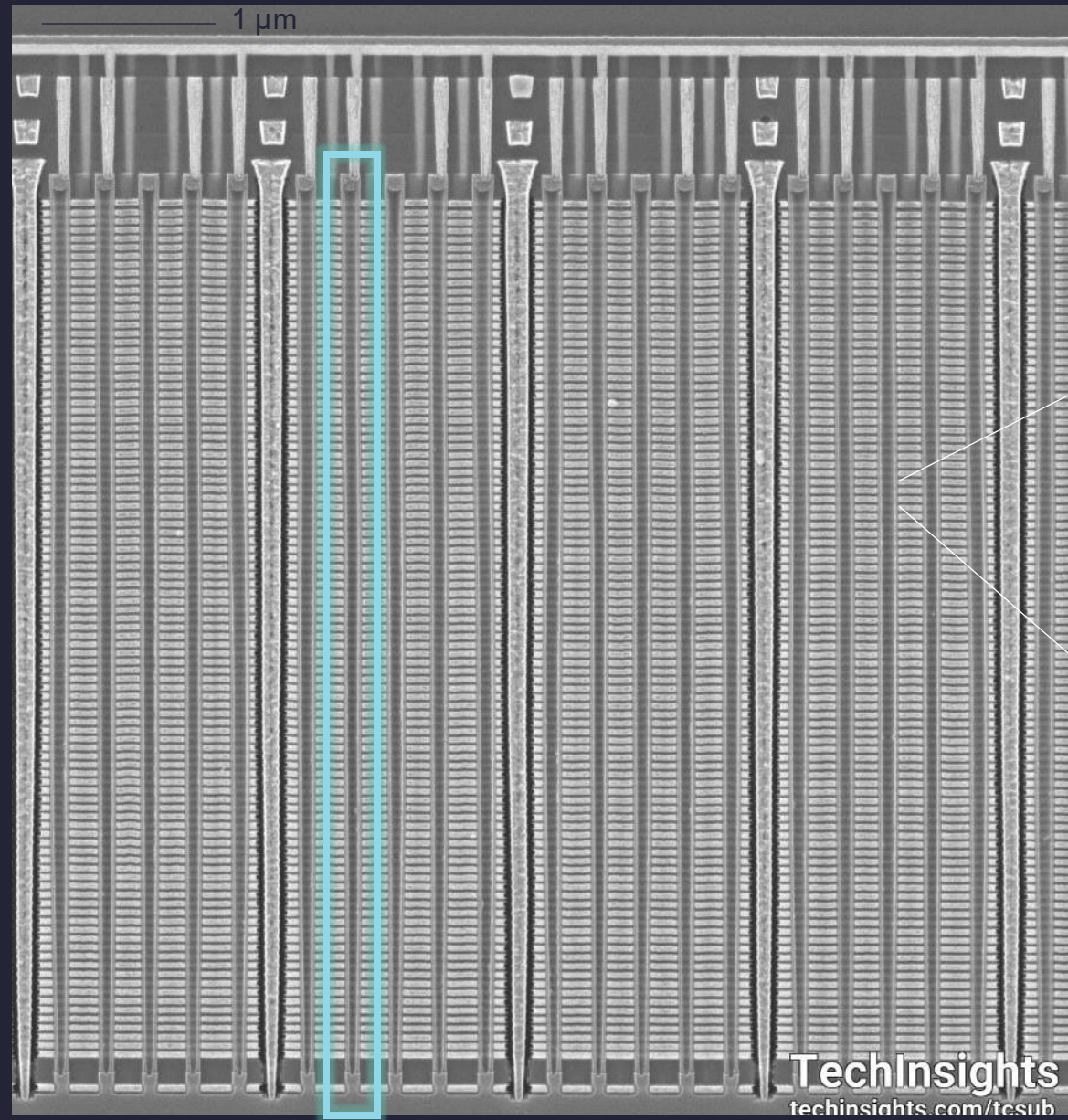
RECIPE

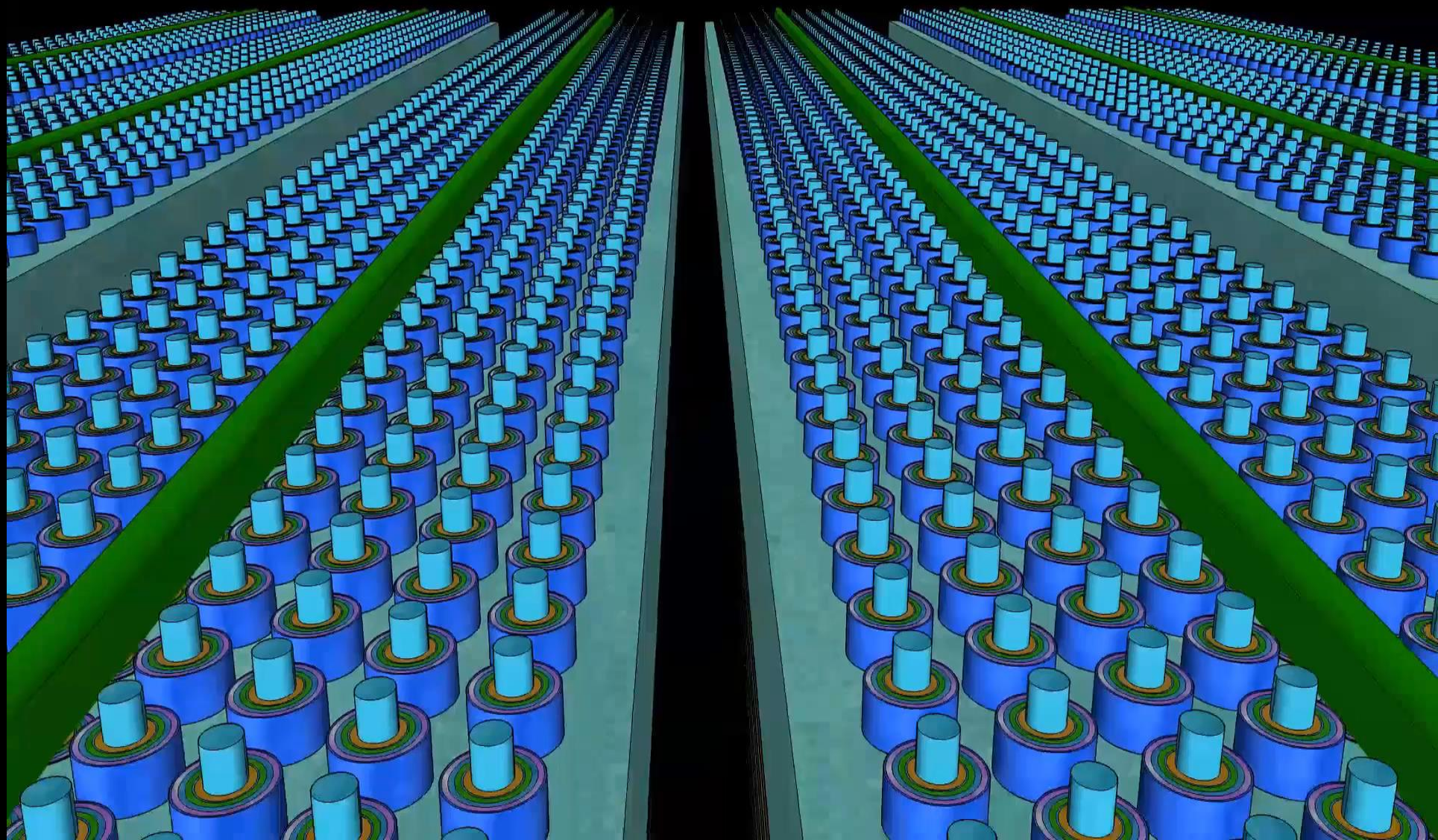


RESULT



Consider memory hole etch in 3D NAND





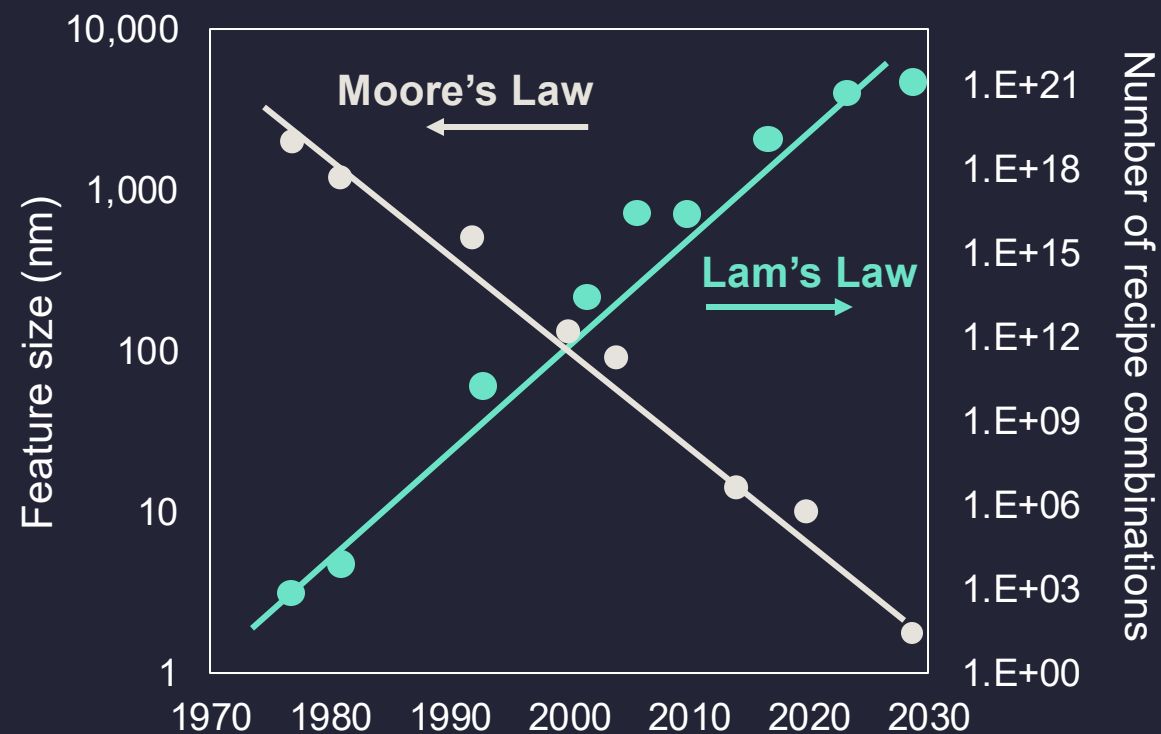


Why not just use a
big data approach?

Simply put,
it costs too
much and
takes too long



Little data
world but *big*
dimensional
space



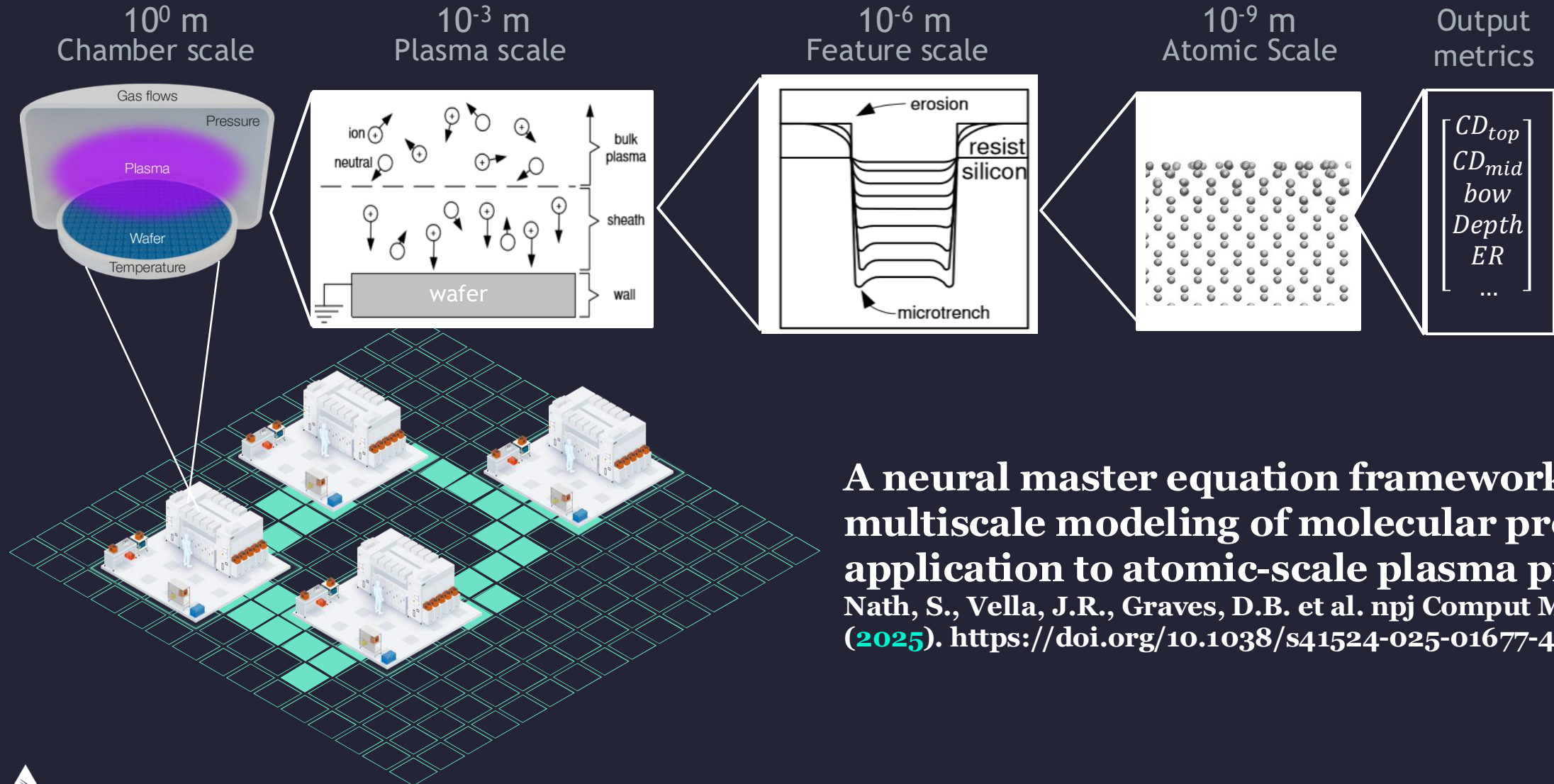
What about
physics?....

$$\mathbf{F} = -\nabla U$$

$$COP_{ideal} = \frac{T_C}{T_H - T_C}$$

$$K = \frac{p^2}{2m}$$

Scales that span at least nine orders of magnitude



A neural master equation framework for multiscale modeling of molecular processes: application to atomic-scale plasma processes

Nath, S., Vella, J.R., Graves, D.B. et al. npj Comput Mater 11, 231 (2025). <https://doi.org/10.1038/s41524-025-01677-4>

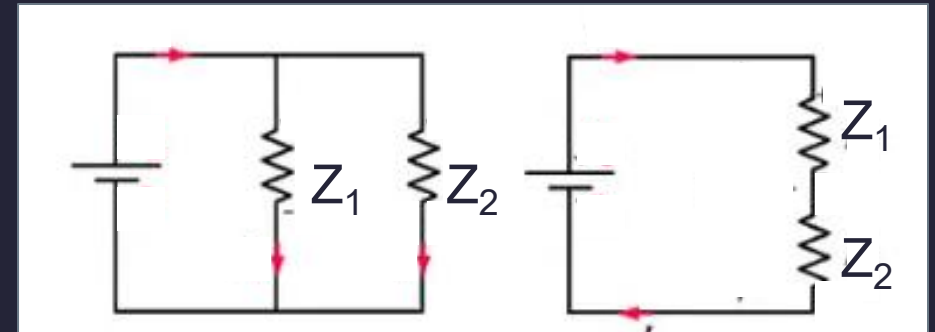
Complexity Reduction and Semi-Empiricism

TABLE I. Oxygen reaction set.

Reaction		Rate coefficients
$e + O_2$	\longrightarrow	$O_2^+ + 2e$ $k_1 = 9.0 \times 10^{-10} (T_e)^2 \exp(-12.6/T_e) \text{ cm}^3 \text{ s}^{-1}$
$e + O_2$	\longrightarrow	$O(^3P) + O(^1D) + e$ $k_2 = 5.0 \times 10^{-8} \exp(-8.4/T_e) \text{ cm}^3 \text{ s}^{-1}$
$e + O_2$	\longrightarrow	$O(^3P) + O^-$ $k_3 = 4.6 \times 10^{-11} \exp(2.91/T_e - 1.26/T_e^2 + 6.92/T_e^3) \text{ cm}^3 \text{ s}^{-1}$
$e + O(^3P)$	\longrightarrow	$O^+ + 2e$ $k_4 = 9.0 \times 10^{-9} (T_e)^{0.7} \exp(-13.6/T_e) \text{ cm}^3 \text{ s}^{-1}$
$O^- + O_2^+$	\longrightarrow	$O(^3P) + O_2$ $k_5 = 1.4 \times 10^{-7} \text{ cm}^3 \text{ s}^{-1}$
$O^- + O^+$	\longrightarrow	$O(^3P) + O(^3P)$ $k_6 = 2.7 \times 10^{-7} \text{ cm}^3 \text{ s}^{-1}$
$e + O^-$	\longrightarrow	$O(^3P) + 2e$ $k_7 = 1.73 \times 10^{-7} \exp(-5.67/T_e + 7.3/T_e^2 - 3.48/T_e^3) \text{ cm}^3 \text{ s}^{-1}$
$e + O_2$	\longrightarrow	$O(^3P) + O(^3P) + e$ $k_8 = 4.23 \times 10^{-9} \exp(-5.56/T_e) \text{ cm}^3 \text{ s}^{-1}$
$e + O(^3P)$	\longrightarrow	$O(^1D) + e$ $k_9 = 4.47 \times 10^{-9} \exp(-2.286/T_e) \text{ cm}^3 \text{ s}^{-1}$
$O(^1D) + O_2$	\longrightarrow	$O(^3P) + O_2$ $k_{10} = 4.1 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$
$O(^1D) + O(^3P)$	\longrightarrow	$O(^3P) + O(^3P)$ $k_{11} = 8.1 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$
$O(^1D)$	(wall)	$O(^3P)$ $k_{12} = D_{\text{eff}}/\Lambda^2 \text{ s}^{-1}$
$e + O(^1D)$	\longrightarrow	$O^+ + 2e$ $k_{13} = 9.0 \times 10^{-9} (T_e)^{0.7} \exp(-11.6/T_e) \text{ cm}^3 \text{ s}^{-1}$
$O^+(g)$	(wall)	$O(^3P)(g)$ $k_{14} = 2 u_{B,O^+} (R^2 h_L + RL h_R) / R^2 L \text{ s}^{-1}$
$O_2^+(g)$	(wall)	$O_2(g)$ $k_{15} = 2 u_{B,O_2^+} (R^2 h_L + RL h_R) / R^2 L \text{ s}^{-1}$
$O(g)$	(wall)	$\frac{1}{2} O_2(g)$ $k_{16} = \gamma_{\text{rec}} D_{\text{eff}} / \Lambda^2 \text{ s}^{-1}$



PARALLEL



$$\frac{1}{Z_{\text{eff}}} = \frac{1}{Z_1} + \frac{1}{Z_2}$$

$$Z_{\text{eff}} = Z_1 + Z_2$$

$$Z_{\text{eff}} \sim Z_1$$

When $Z_2 \gg Z_1$

$$Z_{\text{eff}} \sim Z_2$$

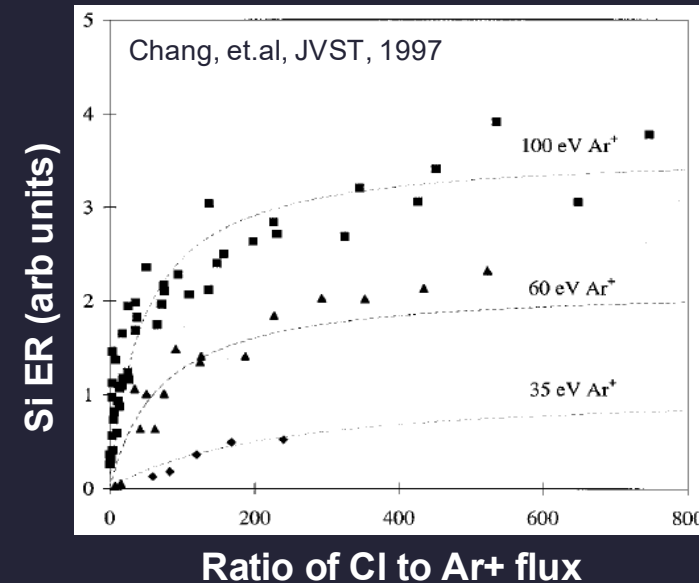
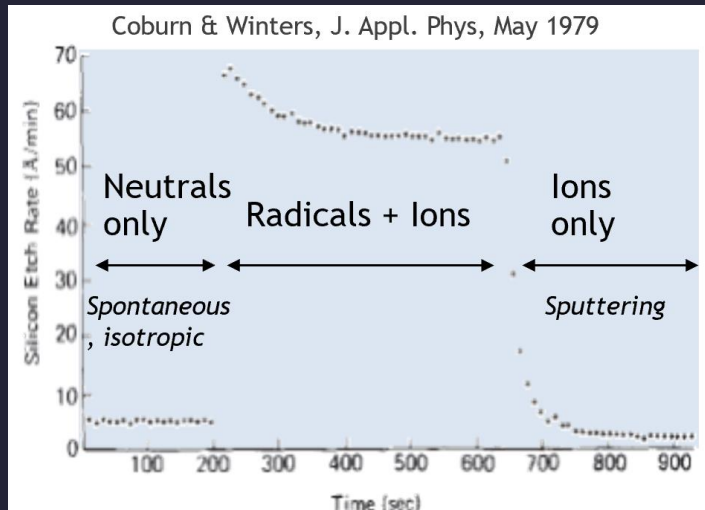
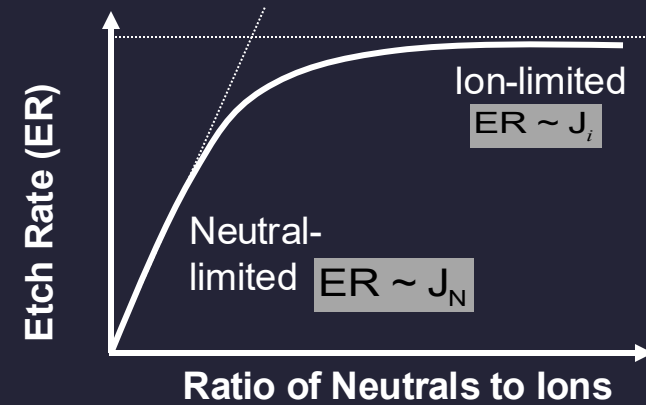
When $Z_1 \gg Z_2$


Where $Z \equiv$ chemical impedance $\sim 1/k_{\text{eff}}$

Basic Plasma Etch Mechanism: Ion-Neutral Synergy

$$\text{Etch Rate} \approx \frac{1}{\frac{U_0}{(\epsilon_i^{1/2} - \epsilon_{th}^{1/2})_i \cdot J_i} + \frac{1}{\nu \cdot S_0 \cdot J_N}}$$

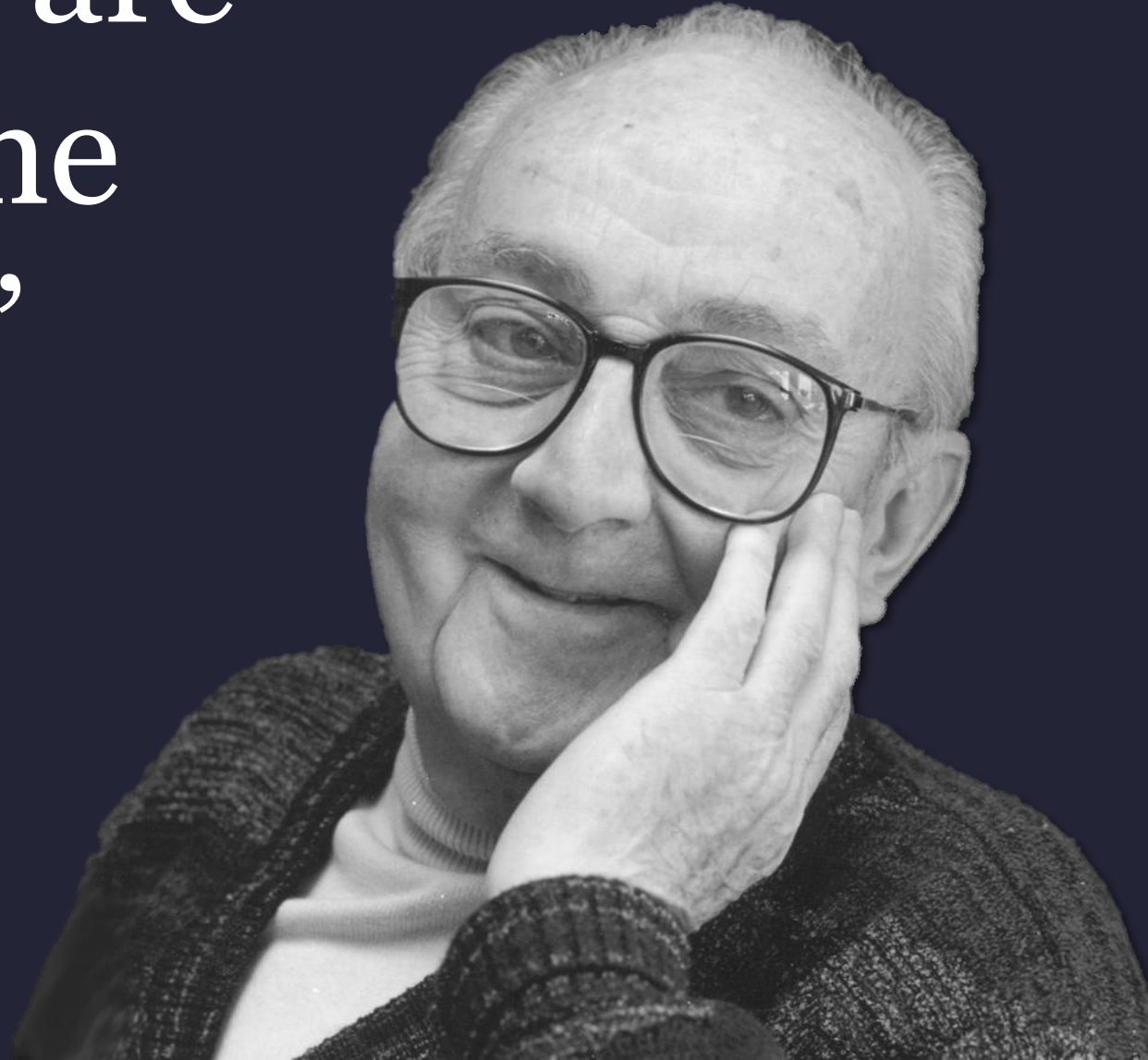
Ion Energy
Ion Flux
Neutral Flux





“All models are
wrong, some
are useful.”

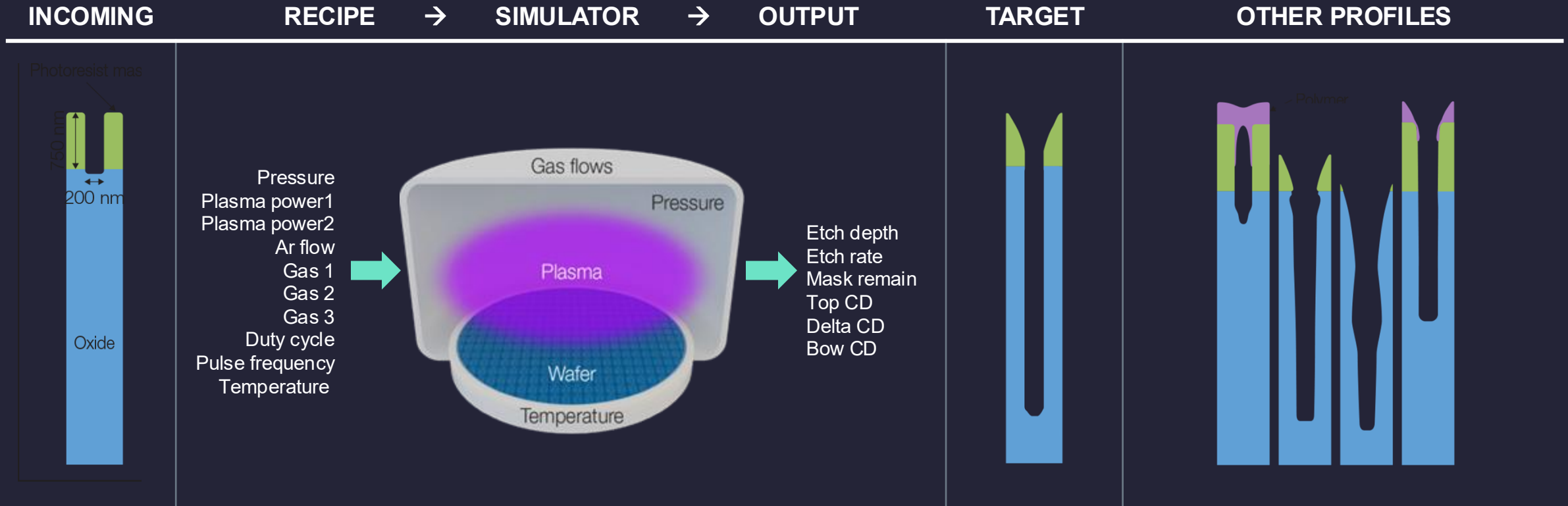
George Box, 1976



Let's play a "game" to benchmark models (and Humans)



A virtual plasma etch process twin

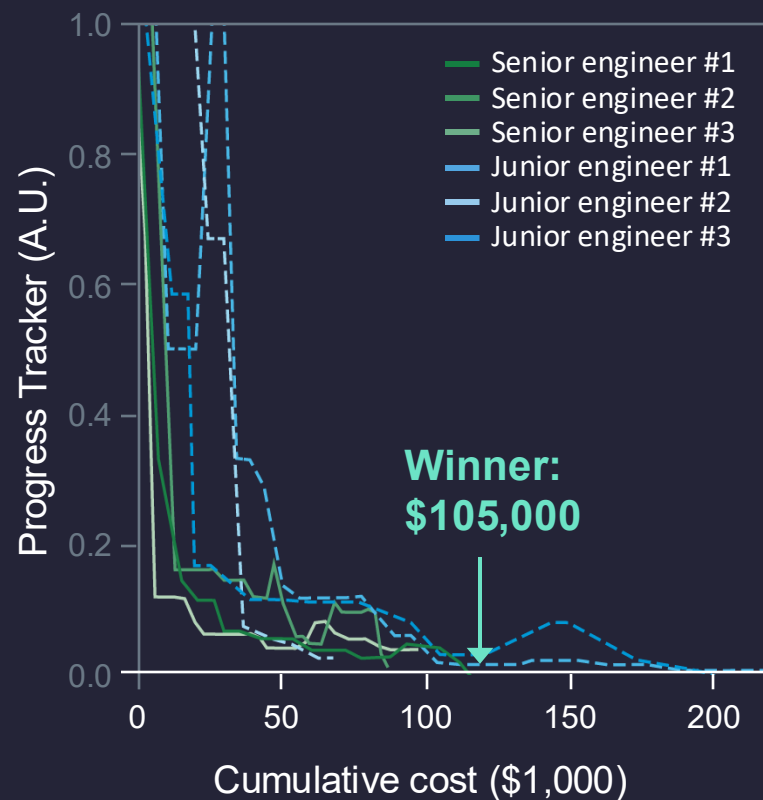


Kanarik, K.J., Osowiecki, W.T., Lu, Y.(*et al.* Human-machine collaboration for improving semiconductor process development. *Nature* **616**, 707–711 (2023). <https://doi.org/10.1038/s41586-023-05773-7>

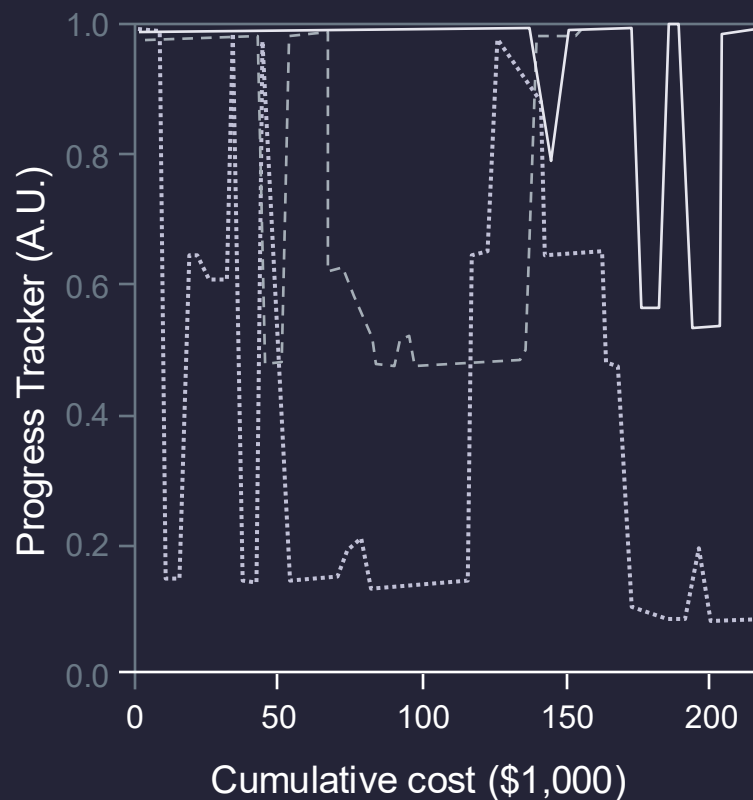


Machine **alone** was no match for expert engineer

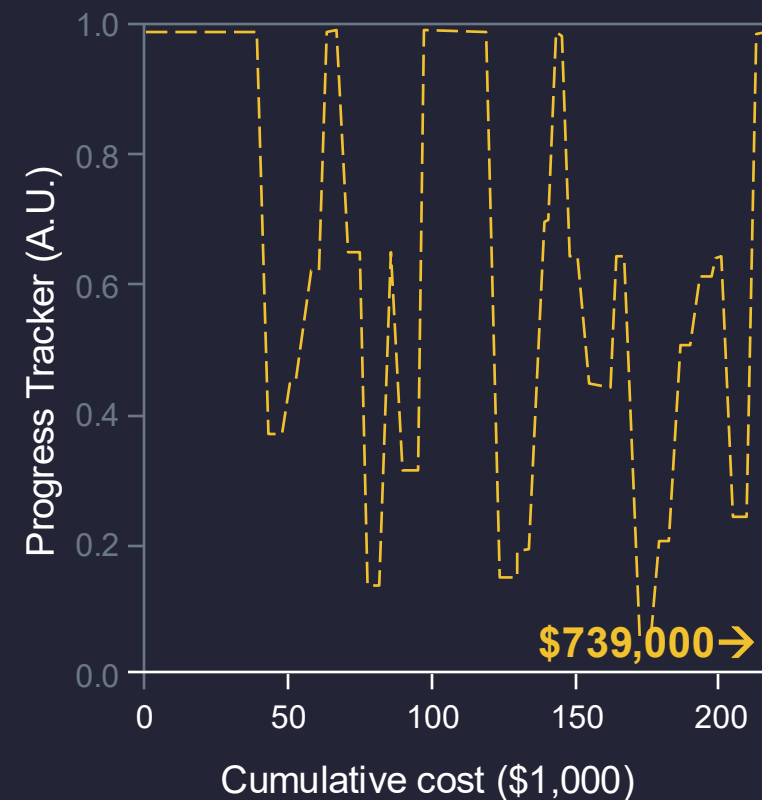
Process engineers



Inexperienced humans

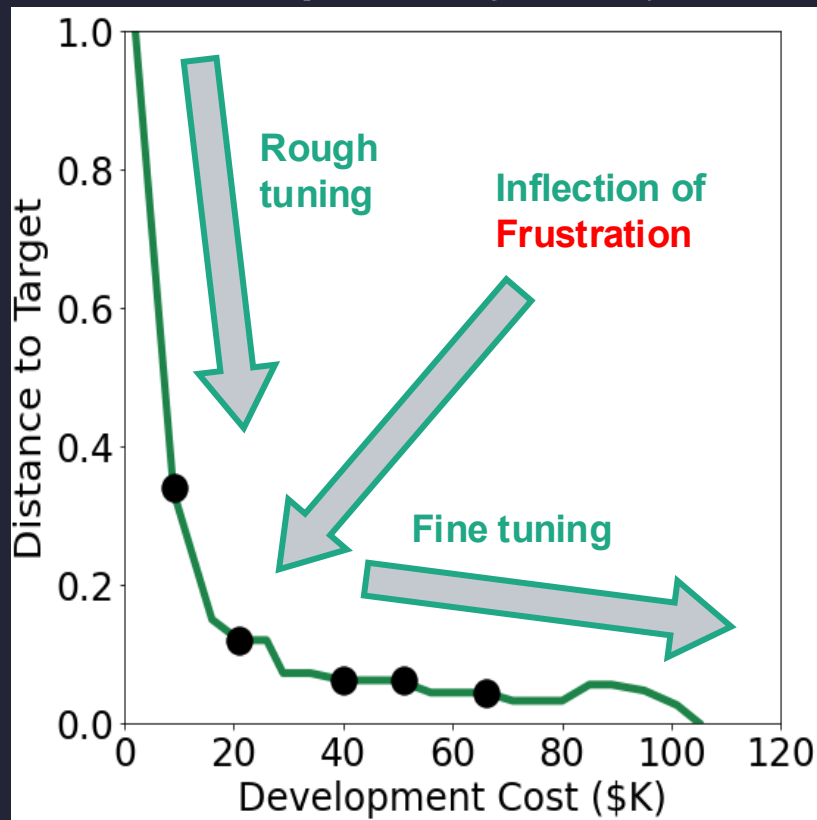


Computer algorithm



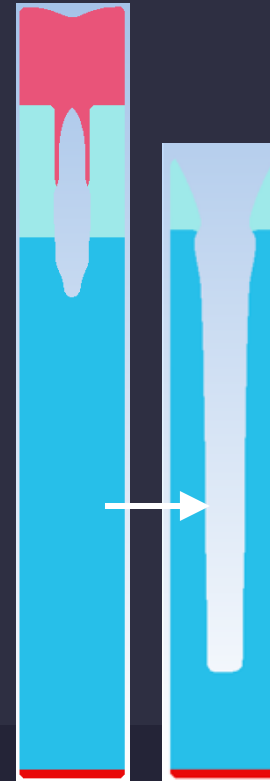
Human learning curve consists of rough and fine tuning

Expert trajectory



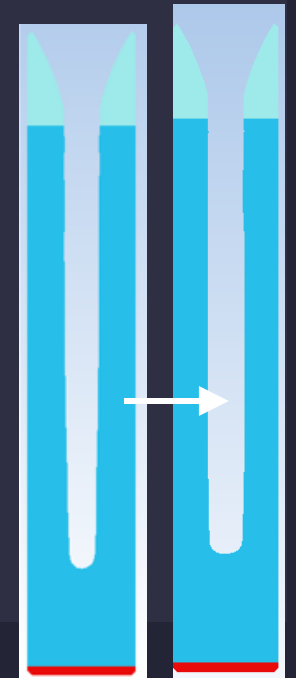
Rough-tuning stage

- Baseline from experience
- Domain knowledge and physical intuition are valuable
- Fulfilling, rapid progress *toward* solution



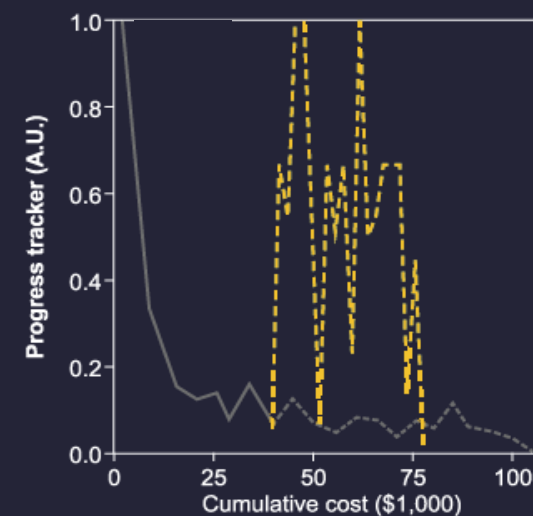
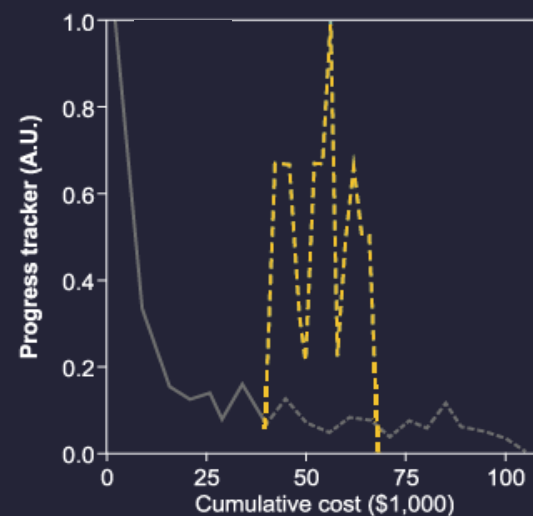
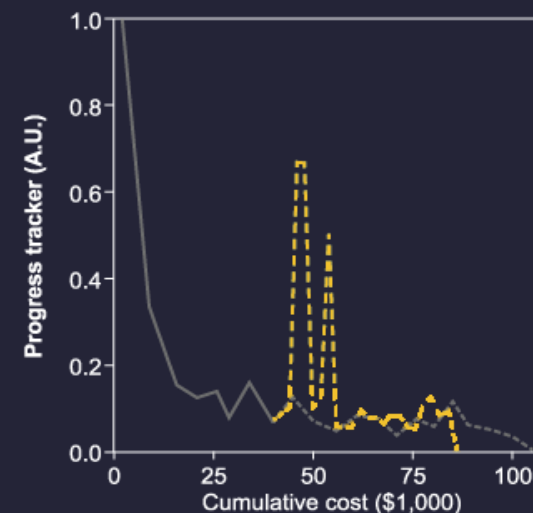
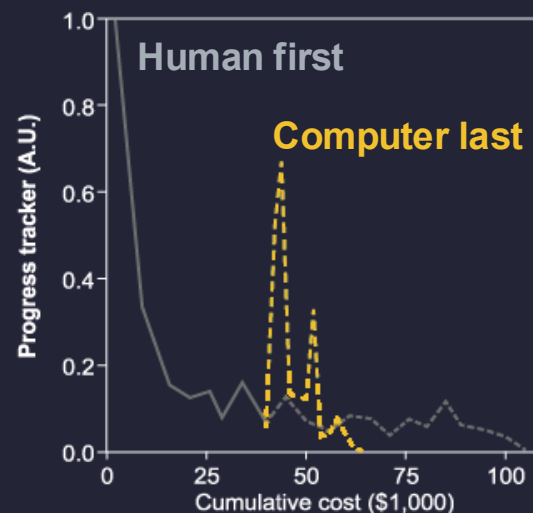
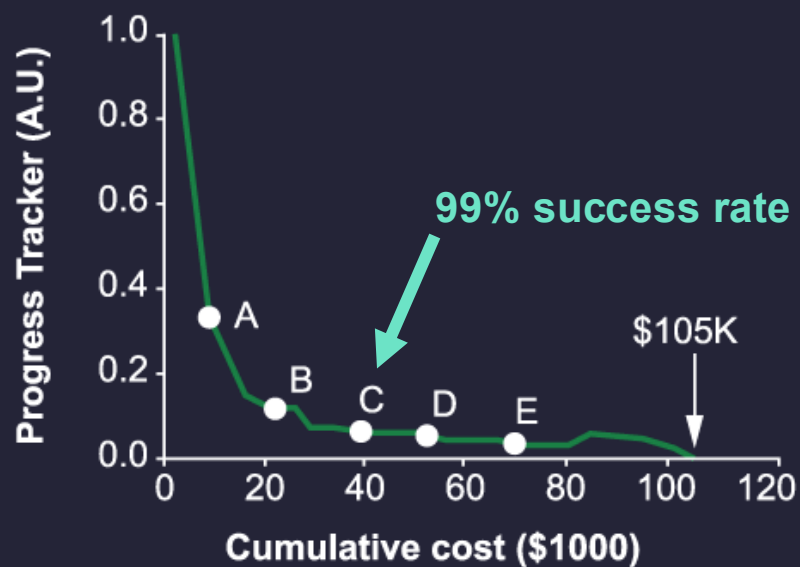
Fine-tuning stage

- Close to spec
- Physical intuition and domain knowledge less useful
- Frustrating, low-productivity path to solution



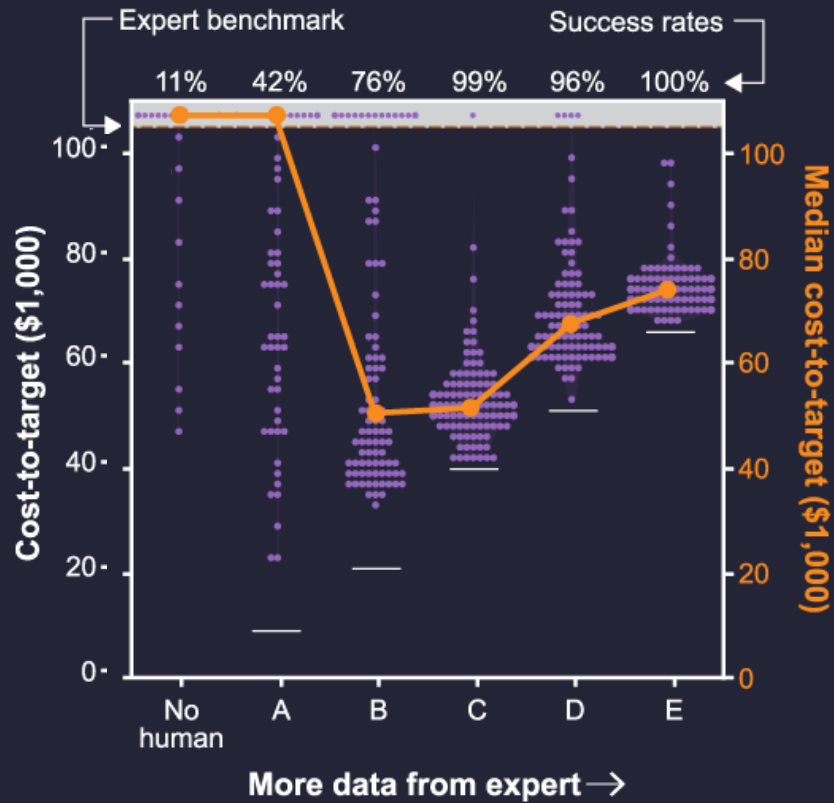
Human-machine collaboration yields cost and time savings

Expert trajectory

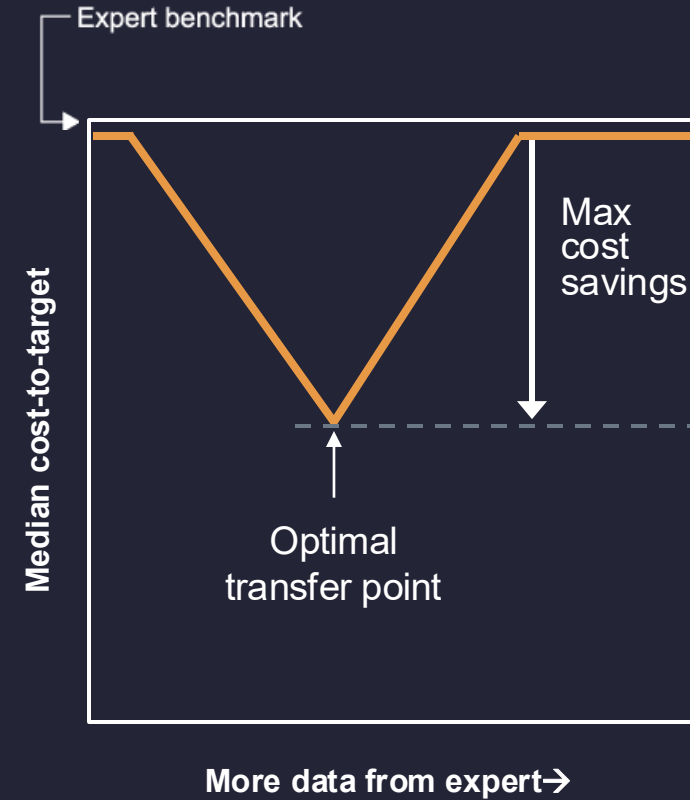


Optimal transfer leverages human investment

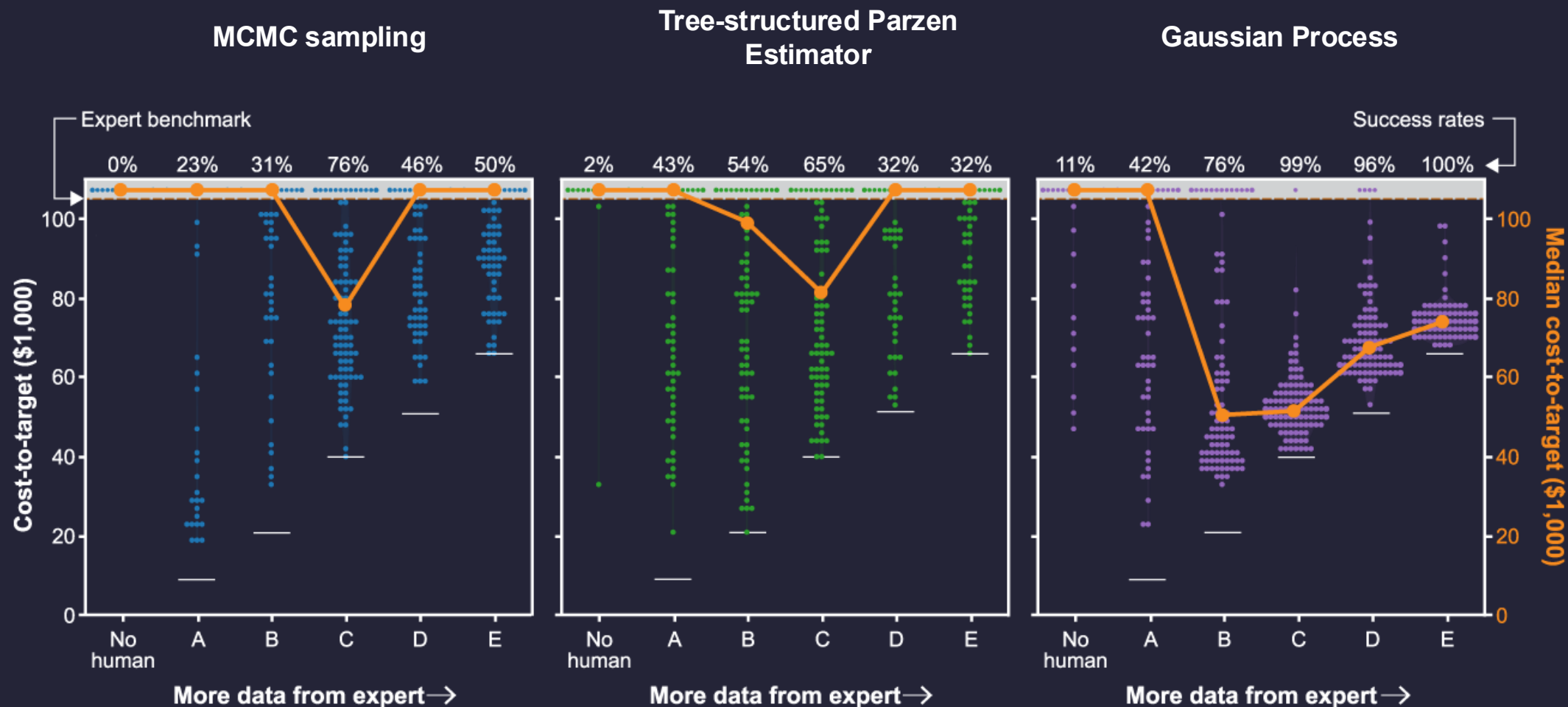
Experimental V-curve



Schematic



Bayesian Optimization Algorithm Comparison



And the winner is...

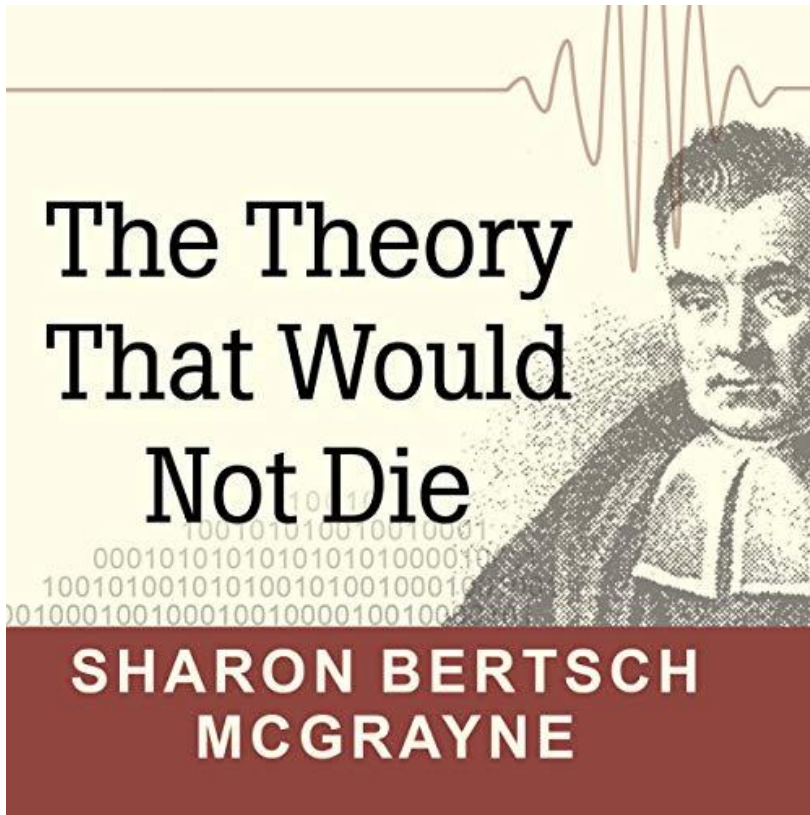
Bayesian Optimization using a Gaussian Process

Görtler, et al., "A Visual Exploration of Gaussian Processes", Distill, 2019.

<https://distill.pub/2019/visual-exploration-gaussian-processes/>

Eric J. Ma, An Attempt At Demystifying Bayesian Deep Learning

<https://ericmjl.github.io/bayesian-deep-learning-demystified/#/IntroductionSlide>



How Bayes' Rule Cracked the Enigma Code, Hunted Down Russian Submarines, and Emerged Triumphant from Two Centuries of Controversy



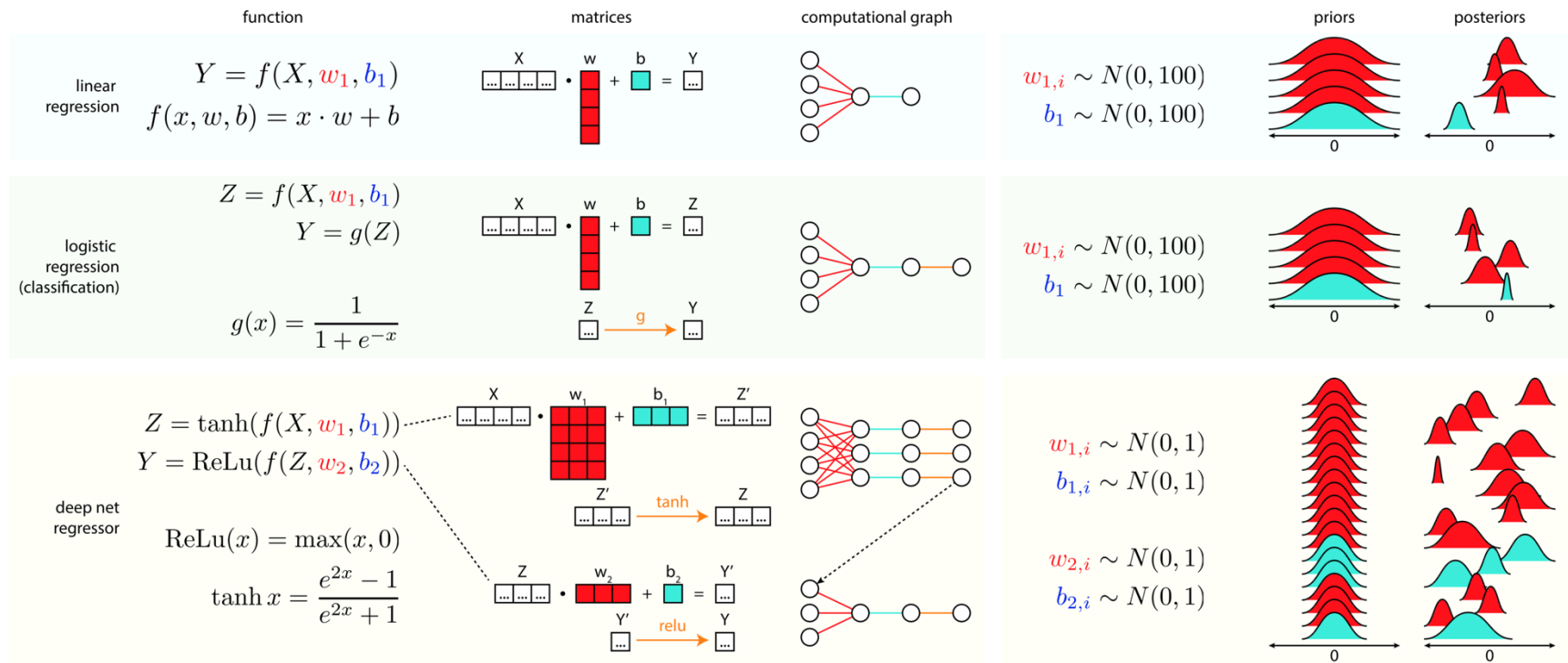
Princeton Plasma Physics School

An Attempt At Demystifying Bayesian Deep Learning

Eric J. Ma

<https://ericmjl.github.io/bayesian-deep-learning-demystified/#/IntroductionSlide>

Cheat Sheet



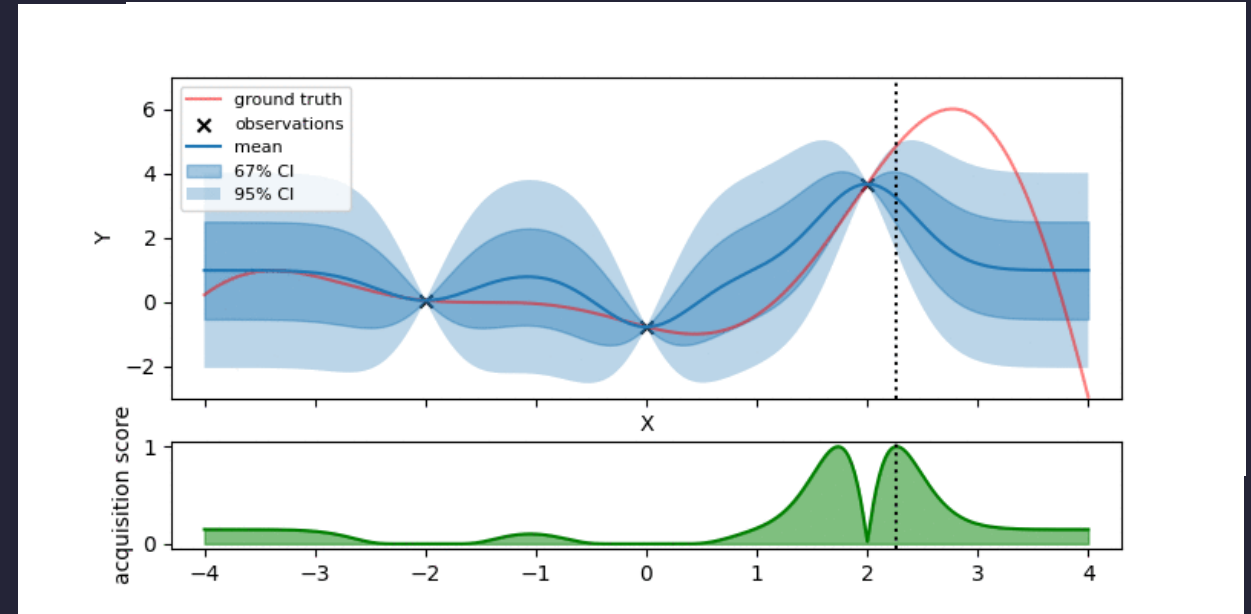
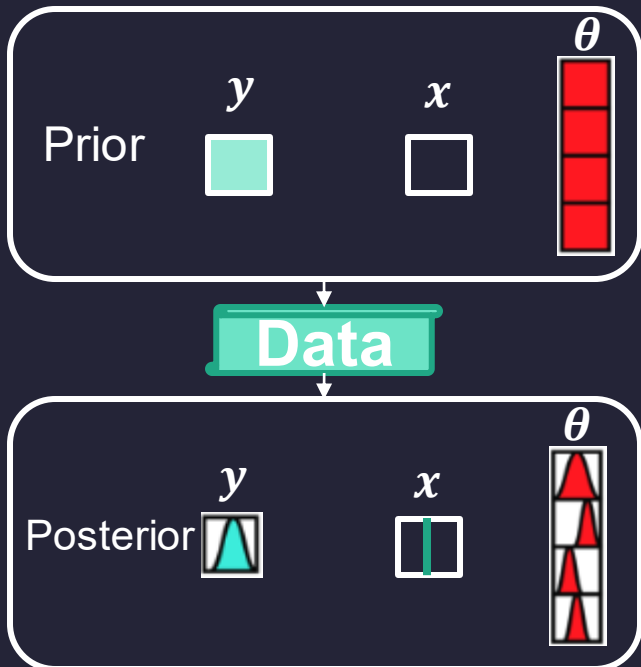
Source: [ericmjl/bayesian-deep-learning-demystified](https://ericmjl.github.io/bayesian-deep-learning-demystified)

Bayesian Optimization

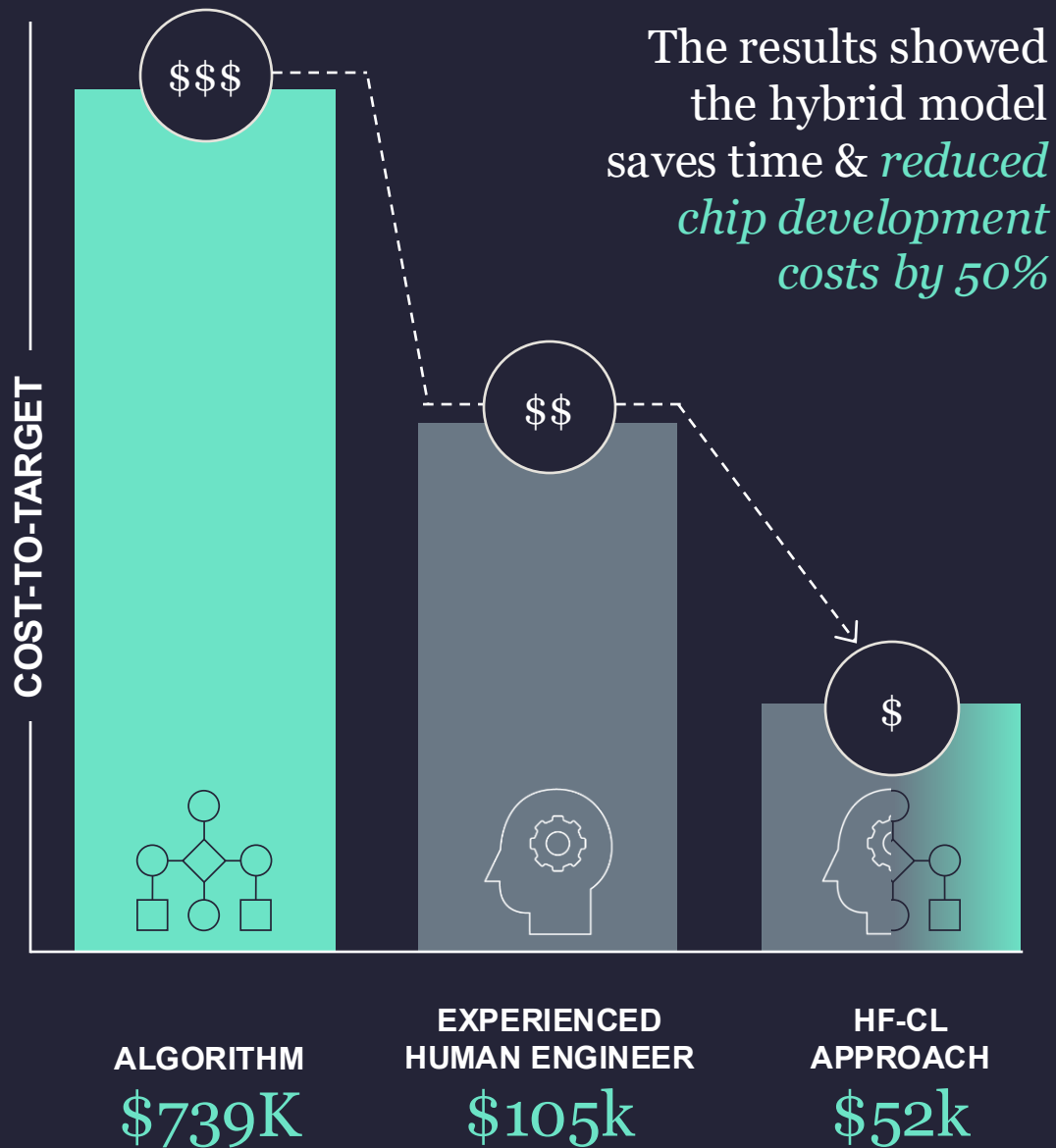
Bayes theorem: $p(\theta|D) = \frac{p(\theta)p(D|\theta)}{p(D)}$

Surrogate: $y = f(x, \theta) + \varepsilon$ ← Noise

Metrology Recipe Model parameters



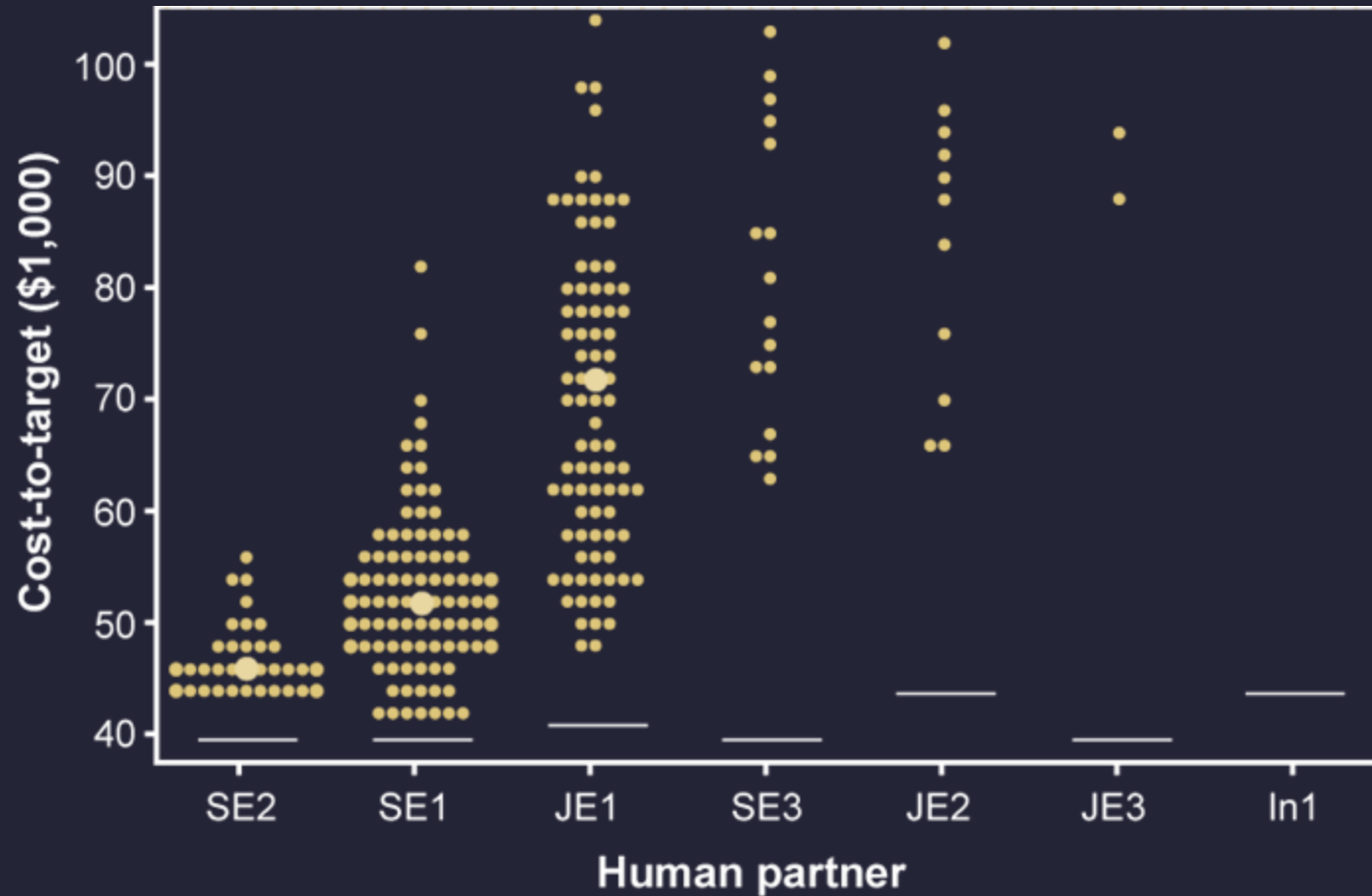
- Bayesian Optimization is a widely adopted ML/AI framework for optimization and inverse design where performance evaluation is costly
 - Bayesian inference allows one to characterize epistemic uncertainty
 - BO makes cost-efficient decisions for next experiment based on evidence collected from existing data and remaining uncertainty of model
 - BO updates the model and experiment decision based on new data



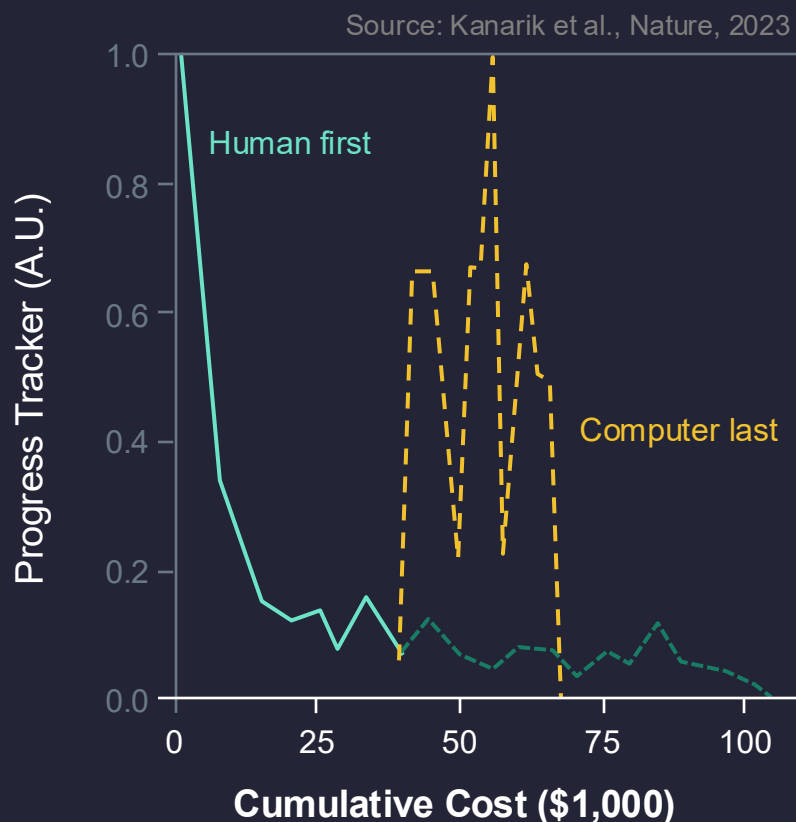
Hybrid approach wins

Human-first,
machine-last
saves countless
hours and
millions of dollars

Computer should partner with an experienced engineer



Algorithm behaves differently than process engineer



Parameter 1	Parameter 2	Parameter 3	Parameter 4	Parameter 5	Parameter 6	Parameter 7	Parameter 8
1148.6	68.5	4026	90.7	33.9	20.9	220.0	50.9
1165.2	66.5	3594	198.7	33.3	22.3	231.0	58.4
1166.8	67.1	3480	167.6	32.6	21.3	226.1	58.2
1149.3	68.3	3842	109.2	30.7	17.9	252.7	58.3
1160.1	60.5	3110	181.0	27.2	17.8	204.5	58.1
1158.0	60.0	3103	156.8	27.0	17.8	202.9	58.0
1143.9	68.6	3550	90.1	33.4	16.1	180.0	59.5
1137.1	67.3	3715	96.7	34.1	17.4	180.6	59.5
1160.5	67.7	3830	169.9	30.2	18.0	199.4	57.0
1170.7	67.0	3728	196.3	29.2	17.5	195.7	56.3
1161.6	67.2	3687	181.9	30.2	17.7	194.5	56.0

There is high value
learning from virtual
worlds that *are not*
precisely predictive

Few-Shot Test-Time Optimization Without Retraining for Semiconductor Recipe Generation and Beyond

<http://arxiv.org/abs/2505.16060>

Shangding Gu^{1*}, Donghao Ying¹, Ming Jin², Yu Joe Lu³, Jun Wang⁴, Javad Lavaei¹, Costas Spanos¹ (May 2025)

We validate MFL on semiconductor plasma etching tasks, where it achieves target recipe generation in just five iterations, significantly outperforming both Bayesian optimization and human experts.

¹UC Berkeley ²Virginia Tech ³Lam Research ⁴UCL

Princeton Plasma Physics School



Physics Informed Machine Learning

Fewer experiments needed

Improved extrapolation

Ensure physics is obeyed!

Physics-Informed Gaussian Processes for Bayesian Optimization

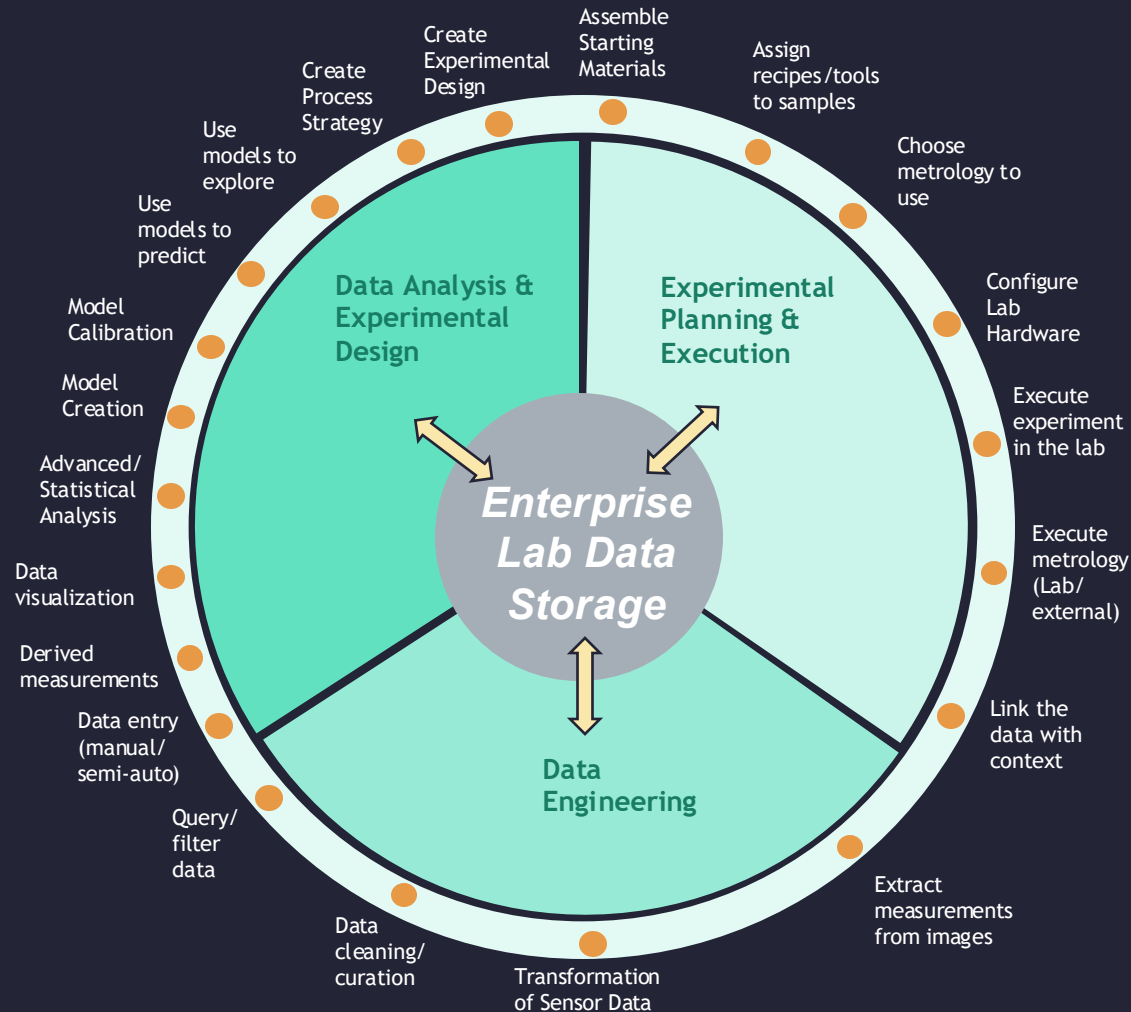
- Additive Models (Data + Physics Residuals)
 - $f(x) = f_{\text{physics}}(x) + f_{\text{residual}}(x)$
 - $f_{\text{physics}}(x)$: physics-based model (PDE, surrogate, empirical)
 - $f_{\text{residual}}(x)$: GP correction
 - Train GP on $y - f_{\text{physics}}(x)$
 - Total prediction = physics model + GP-predicted residual
- Informed Kernels
 - Embed constraints: periodicity, conservation laws, symmetries
 - Example: Periodic kernel: $k(x, x') = \sigma^2 \exp(-2 \sin^2(\pi|x-x'|/p)/l^2)$
 - Learn a composite kernel that combines a physics-informed part and a flexible part.
- Physics-Based Priors
 - Default GP: $\mu(x) = 0$
 - Replace with $\mu(x) = f_{\text{physics}}(x)$
- Physics-Informed Acquisition Functions
 - Guide exploration to physics-interesting areas
 - Feasibility-aware acquisition

Three Approaches to Physics-Informed ML

	Physics-Informed Neural Networks (PINNs)	Physics-Informed Gaussian Processes (PIGPs)	Physics-Informed Neural Operators (PINOs)
Physics incorporation	Penalize PDE residuals in loss function	Embed physics in prior mean/kernels or residuals	Embed PDE constraints into operator learning
Uncertainty quantification	No (unless Bayesian PINNs)	Yes	Not standard
Data requirement	Moderate to high	Low	High
Strengths	Handles complex nonlinear PDEs, flexible	Excellent in data-scarce regimes, principled uncertainty	Learns solution operators across PDE families
Computation	Optimization (can be costly, especially with stiff PDEs)	GP regression (scales poorly with data size)	Requires large training data + compute

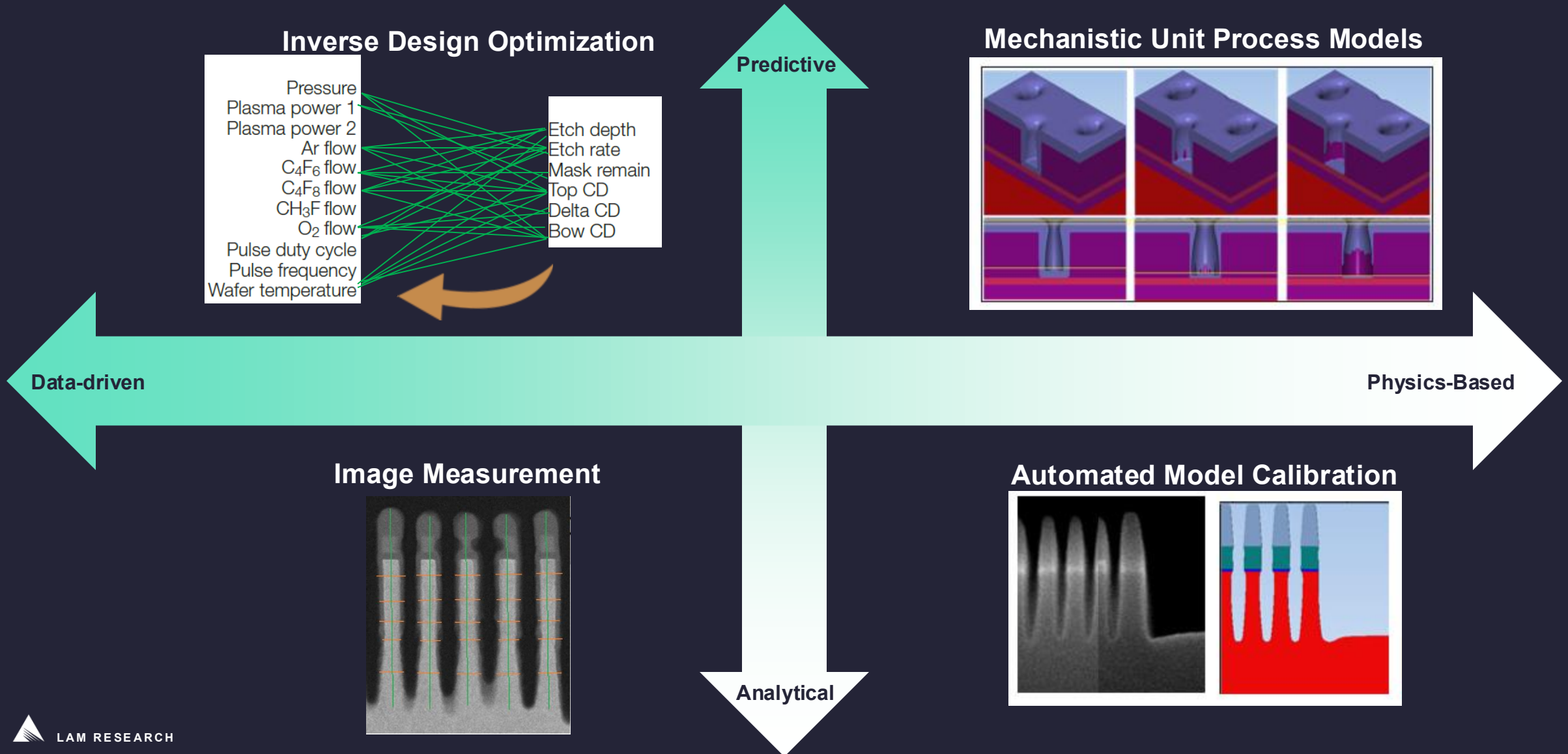
Virtual Process Development

Transform process development through digitalization, automation, simulation & data analysis



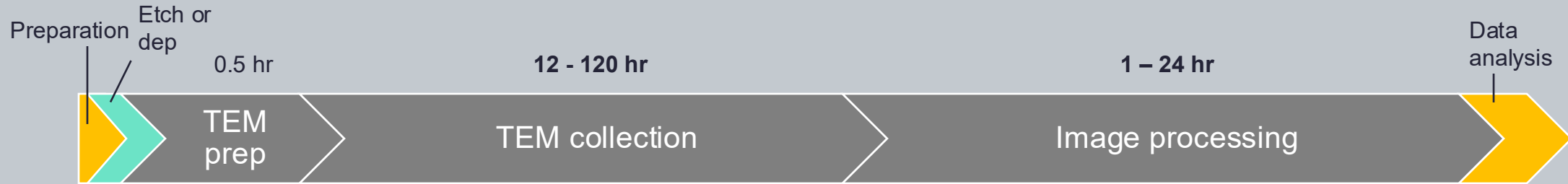
- Process Development is not one monolithic workflow. It is many different paths through a variety of different activities. Catering to these varied workflows requires a **holistic strategy**.
- The activities largely reside in three disciplines, with specific requirements, and must be **connected through enterprise-scale storage of experimental process data**.
- Modernizing and **automating** physical experimental activities in the lab is key to delivering the contextual data to the data store
- Image analysis and **flexible platforms for data science**, machine learning and advanced analytics are critical for data engineering.
- Connecting platforms and systems to create efficient, friction-free workflows = **Virtual Process Development**

Virtual Process Development – Physics and Data

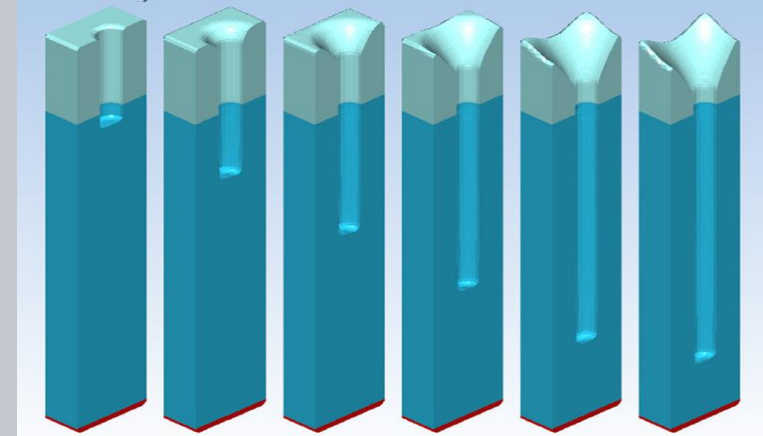


Real-time profile metrology for *100x* cycle time reduction

Metrology for high aspect ratio solution development **costly, time-consuming, and destructive**



Real-time metrology offers *100x* cycle time reduction



Barriers: Business model and some invention required

New Materials Development

- DFT/AI predictions of stability and transition states
- Synthesis has been a bottleneck, but...
 - Combinatorial techniques combined with automation and *autonomy* is revolutionizing the pace of new materials innovation
- Process integration and device fabrication remain bottlenecks





Artificial Intelligence and Machine Learning for Materials Discovery, Synthesis and Characterization

The use of artificial intelligence, including machine learning, is rapidly rising in all areas of materials science, from materials discovery, synthesis, characterization, and performance. This special collection explores these areas and highlights successes and challenges.

Guest Editors:

Parag Banerjee, University of Central Florida

Jeffrey Elam, Argonne National Laboratory

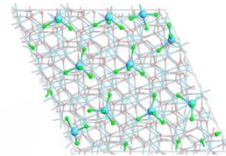
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Editor:

Amy Walker, University of Texas at Dallas

Image Credit: S. Kondati Natarajan, J. Schneider, N. Pandey, J. Wellendorf, and S. Smidstrup, JVST A 43, 033404 (2025) doi.org/10.1116/6.0004288.



Thin Films

[Analysis of x-ray emission spectroscopy \(XES\) data using artificial intelligence techniques included in the XES Neo package](#)

Alaina Humiston; Miu Lun Lau; Tim Stack; Evan Restuccia; Alberto Herrera-Gomez; Min Long; Daniel T. Olive; Jeff Terry

<https://doi.org/10.1116/6.0004326>



Epitaxial Growth of Materials

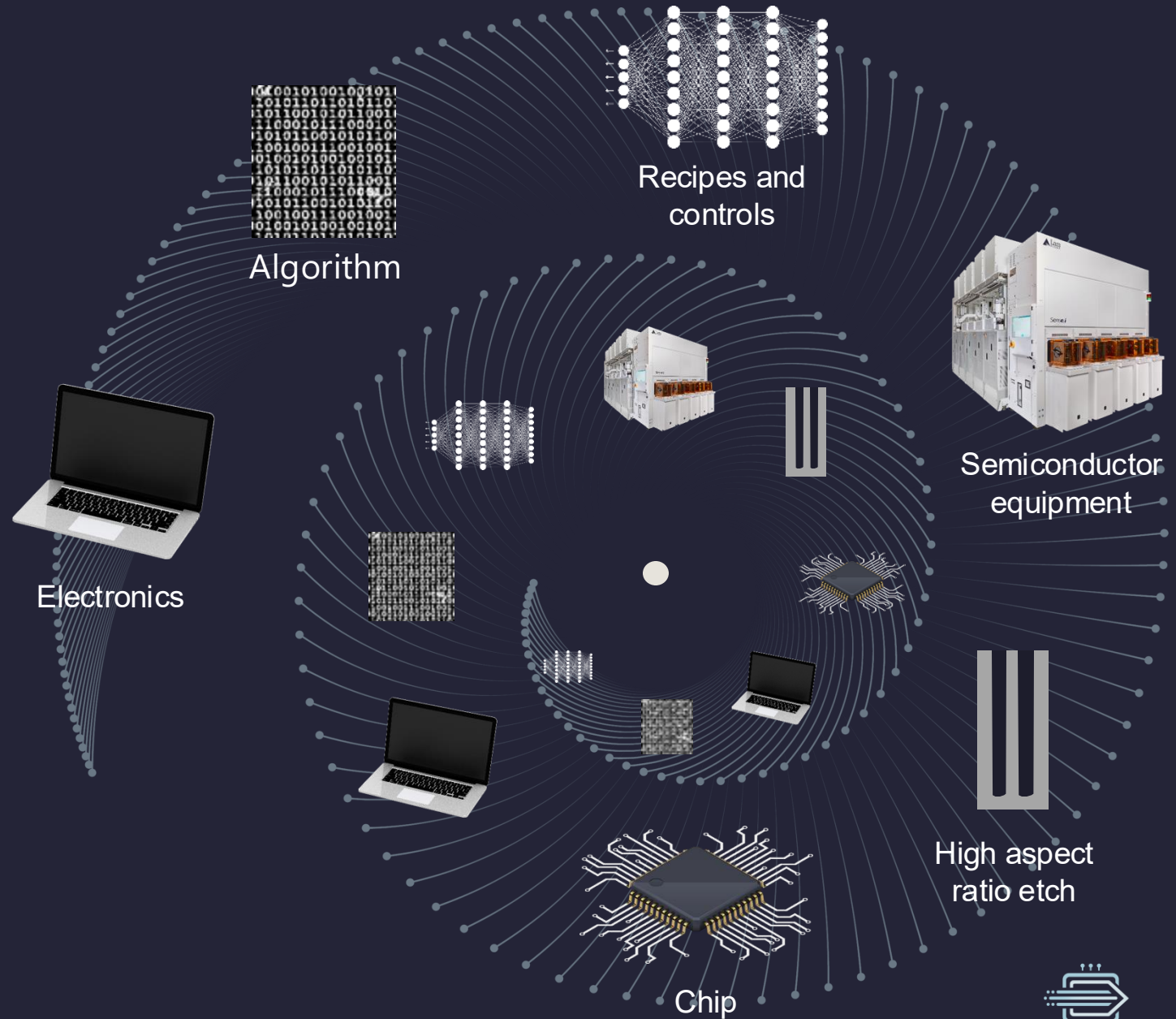
[AI-guided frame prediction techniques to model single crystal diamond growth](#)

Rohan Reddy Mekala; Arjun Srinivasan; Matthias Muehle; Elias Garratt; Adam Porter; Mikael Lindvall

<https://doi.org/10.1116/6.0004290>

Focus	Count
Synthesis	I
Characterization/Analysis	IIII
Monitoring/Control	IIII
Discovery	I

What goes
around comes
around **faster**
and **better**



Further reading

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