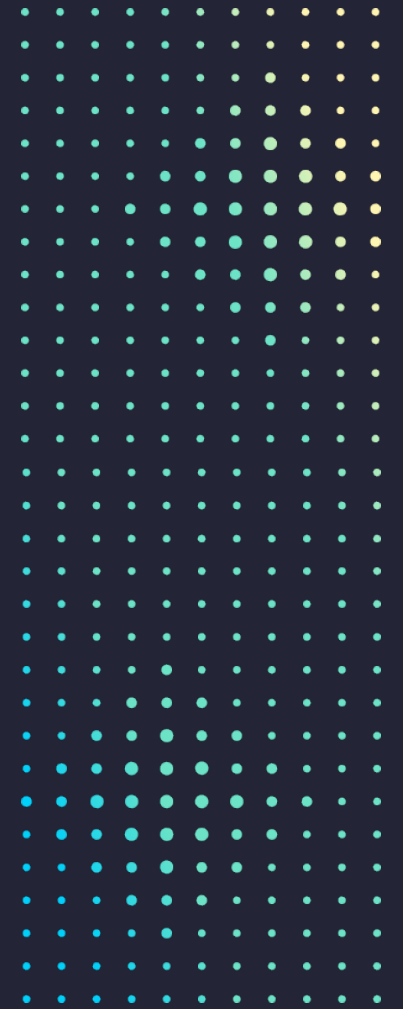


The Power of Virtual Process Development

*Faster solutions, lower cost, workforce
development*

Richard A. Gottscho, Ph.D.

Executive Vice President, Strategic Advisor to the CEO, Innovation Ecosystem



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

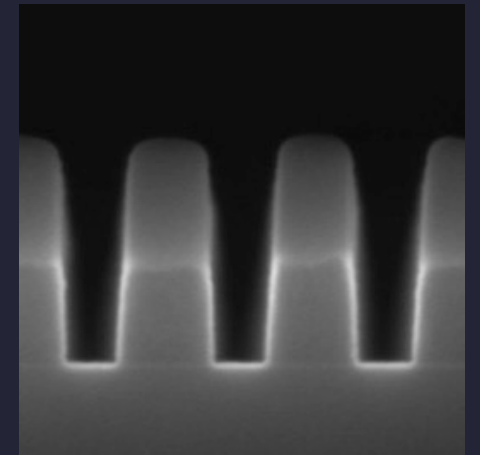
SPEC



RECIPE



RESULT





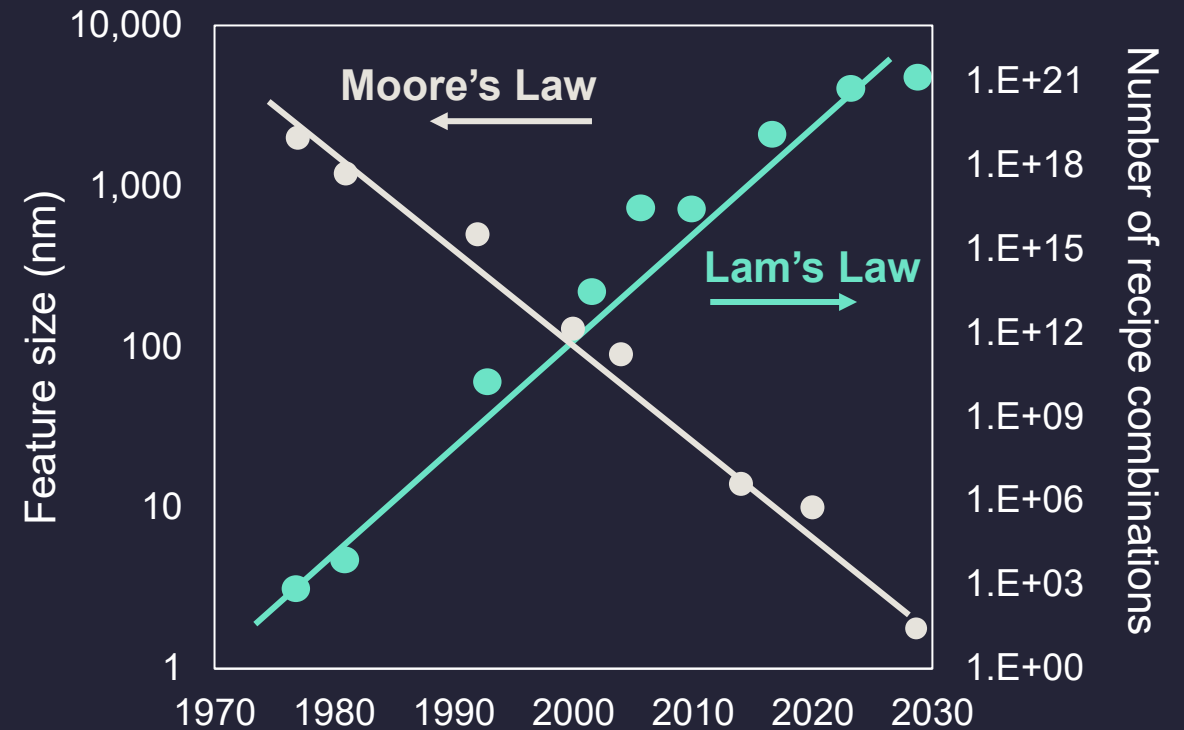
Why not just use a
big data approach?

Simply put,
it costs too
much and
takes too long



Little data
world but *big*
dimensional
space

~ AVOGADRO'S NUMBER OF RECIPES



What about
physics?...

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

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

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

$$P = \frac{dW}{dt}$$

$$p = mv$$

$$\delta E = \int ds = \dots$$

7

8

6

6

2

18

6

7

7

6

9

9

9

3

3

8

5

5

8

9

3

9

9

9

9

9

9

Natural simplifications

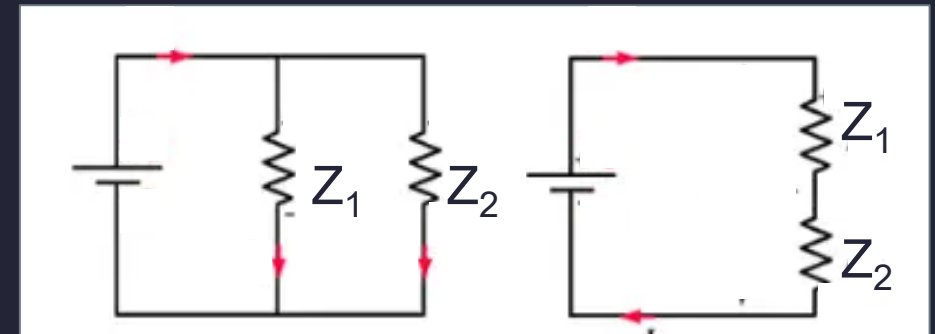
TABLE I. Oxygen reaction set.

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



PARALLEL

SERIES



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

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

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

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

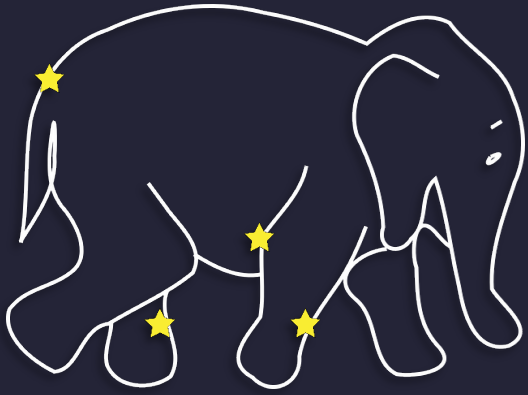
When $Z_2 \gg Z_1$

When $Z_1 \gg Z_2$

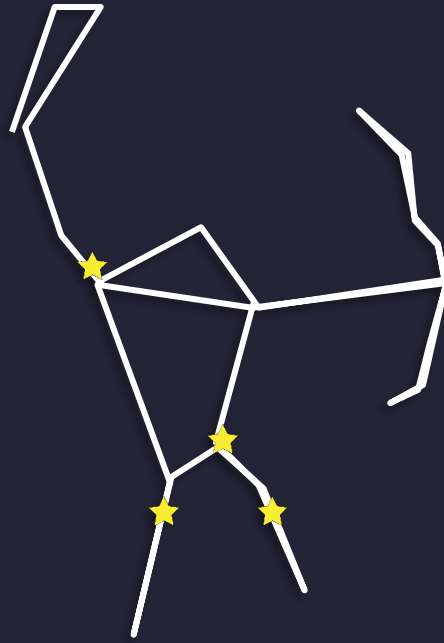
Where $Z \equiv$ chemical impedance $\sim 1/k_{\text{eff}}$

Exploit **little data** with right (physics-based) model

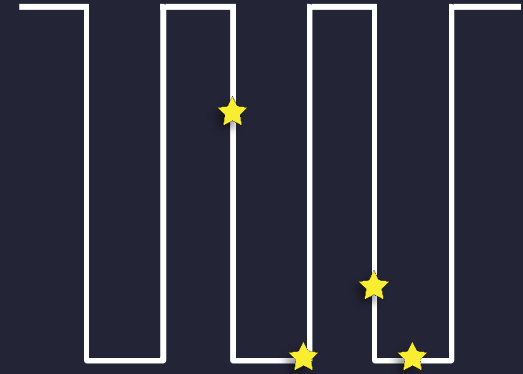
MODEL 1



MODEL 2




MODEL 3



"With four parameters I can fit an elephant, and with five I can make him wiggle his trunk."

*John von Neumann, as related by Freeman Dyson (2004)
"A meeting with Enrico Fermi," Nature 427 (6972)*



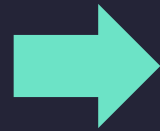
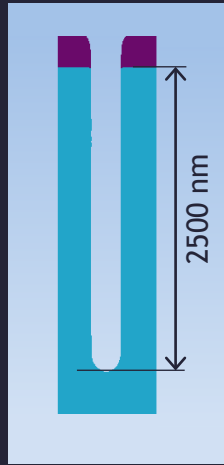


“All models are
wrong, some
are useful.”

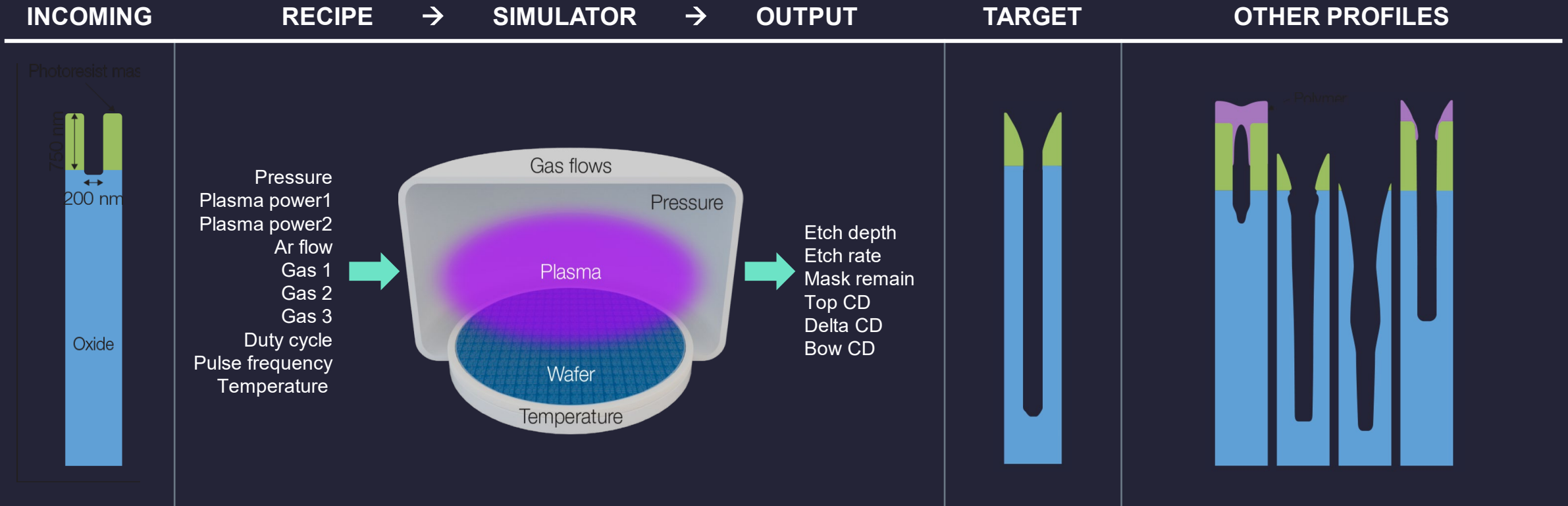
George Box, 1976



Let's play a "game" to benchmark different AI (and human) approaches

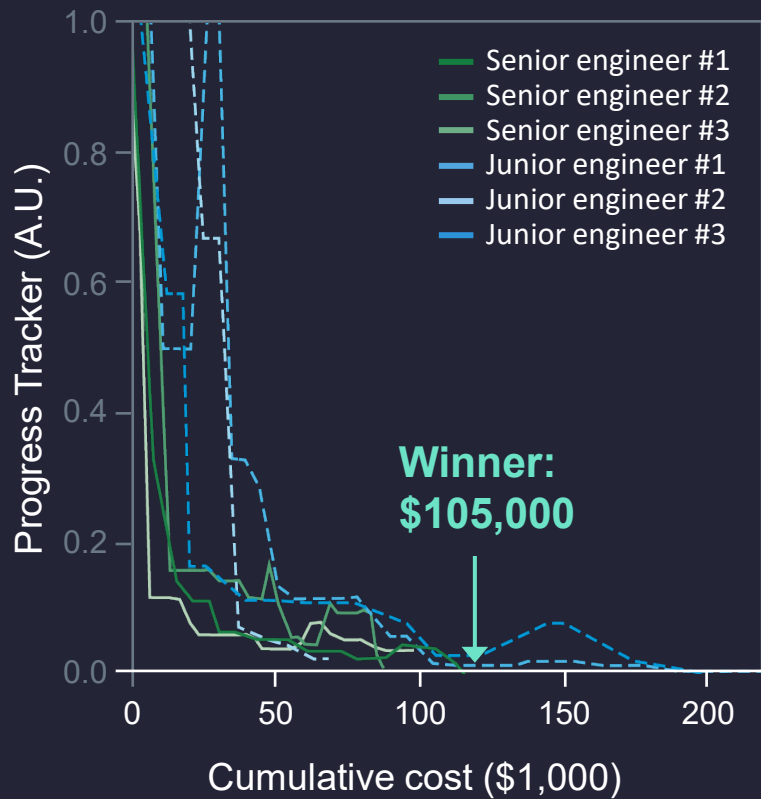


A virtual plasma etch process “cousin”

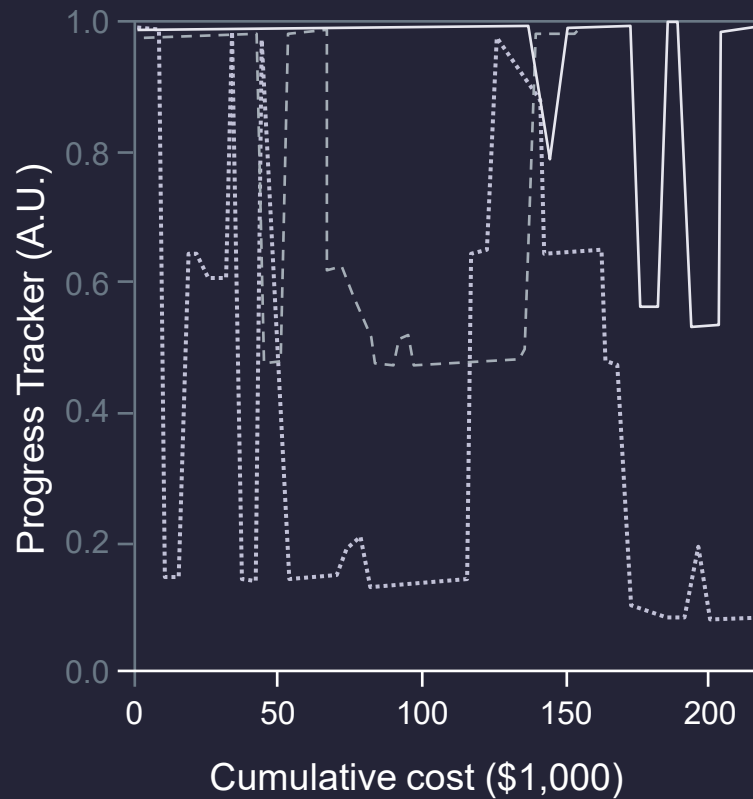


Machine **alone** was no match for expert engineer

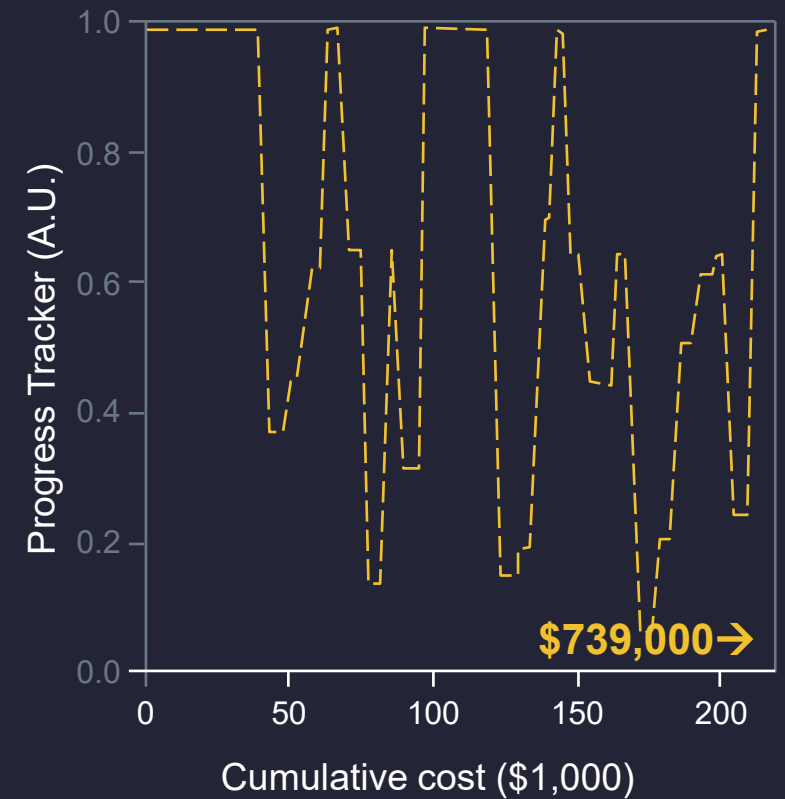
Process engineers



Inexperienced humans

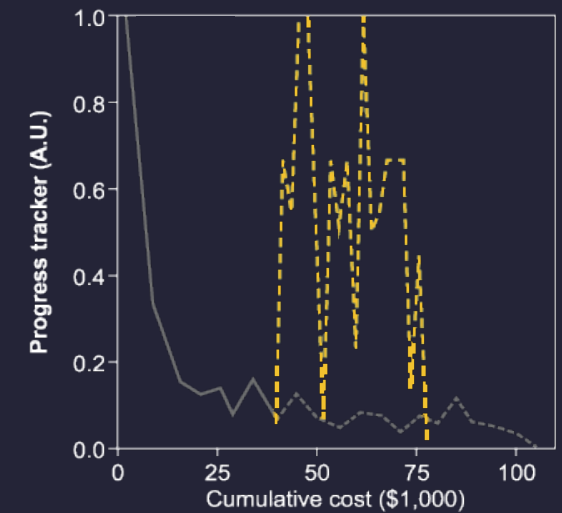
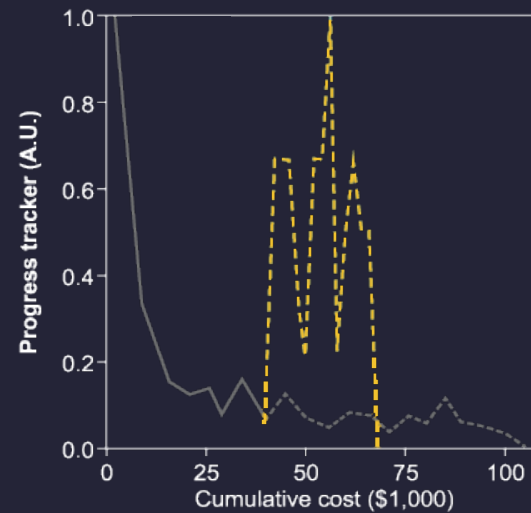
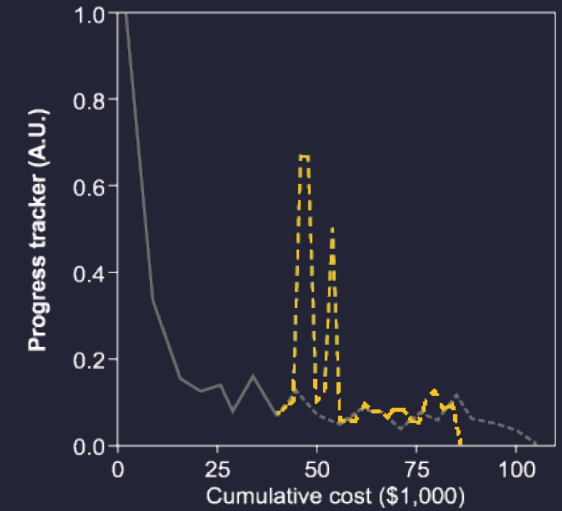
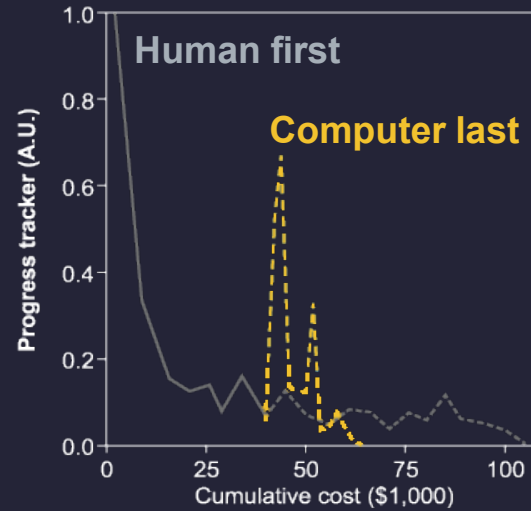


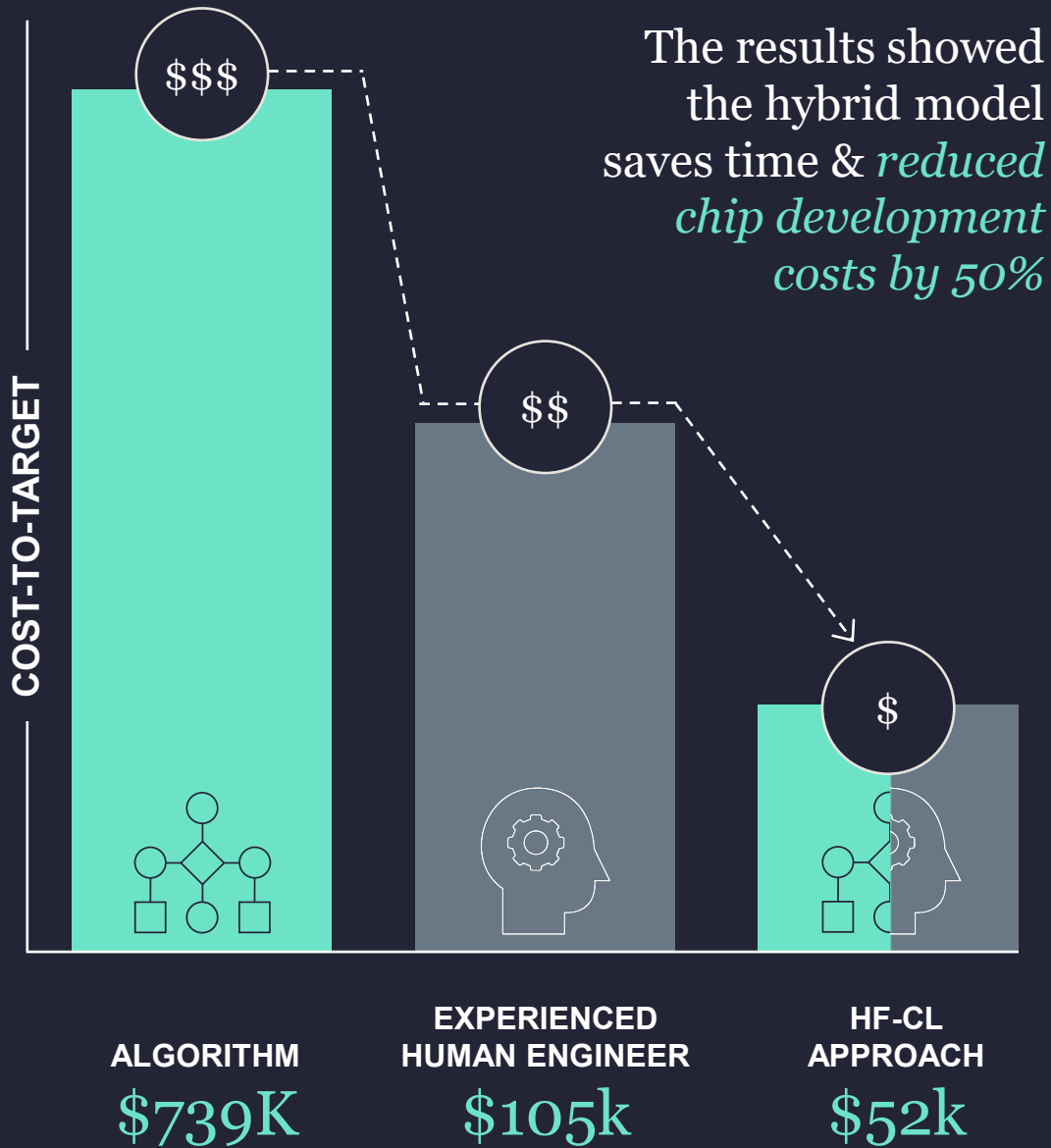
Computer algorithm



Human-machine collaboration yields cost and time savings

Expert trajectory





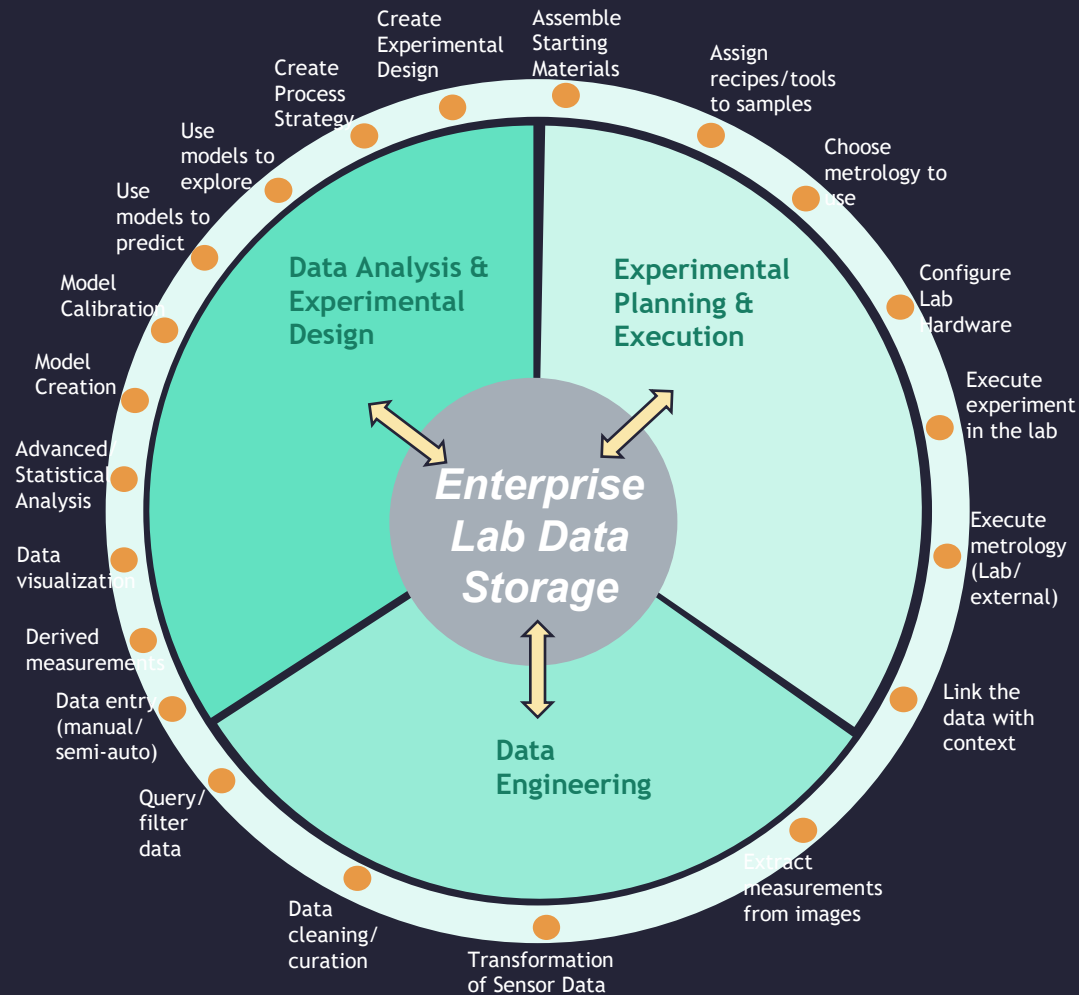
Hybrid approach wins

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

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

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**



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