Artificial Intelligence in Chemical Engineering:

Past, Present, and Future

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AI in Chemical Engineering

- But AI in ChE in not new!
  - Has a 35-year-old literature: >3000 papers
- Highlights of AI in ChE: 1980s to Present
- Identify current challenges and opportunities
  - Conceptual, Implementation, Organizational
- Broad overview
  - Not a detailed technical presentation
  - More details in my paper

The Promise of Artificial Intelligence in Process Systems Engineering: Is it here, finally?
V. Venkatasubramanian, *AIChE Perspective Paper*, Feb 2019

What is AI?

"Artificial Intelligence is the study of how to make computers do things at which, at the moment, people are better."

E. Rich, Artificial Intelligence (1983)

Four Phases of AI in ChE

AI in ChE: Phase I (~1983 – ~2000)

- **Expert Systems Era: Era of Symbolic AI**

Key ideas
- Separation of domain knowledge from inference
- Flexible execution order of program
- IF-THEN Rules for Procedural Knowledge
- Semantic networks for Taxonomies

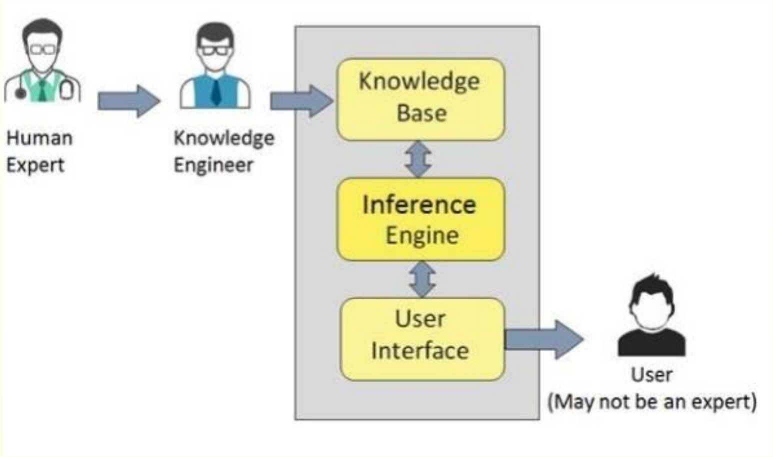


Image source:
ttps://www.tutorialspoint.com/artificial_intelligence/artificial_intelligence_expert_systems.htm

MYCIN: Expert system for diagnosing infectious diseases (1972-82)
- Stanford Computer Science and Medical School Project
- Knowledge base: ~600 rules
- Diagnosed better than the physicians

AI in ChE: Phase I
Expert Systems (~1983 - ~2000)

• CONPHYDE (1983)	Westerberg: Thermodynamic Property Prediction
• DECADE (1985)	Westerberg: Catalyst Design
• MODEX (1986)	Venkatasubramanian: Fault Diagnosis
• DESIGN-KIT (1987)	Stephanopoulos: Process Design
• DSPL (1988)	Davis: Distillation Column Design

- First course on AI in ChE was taught at Columbia (1986-88, Columbia; 1989 – 2011 at Purdue)
    - Venkatasubramanian, V., Artificial intelligence in process engineering: Experiences from a graduate course. *Chem Eng Educ*., 188-192, 1986.
- First conference on AI in ChE was held at Columbia (1987)

ASM (1995 – 2000)

NIST AEGIS Program

Ohio State (Davis)

Purdue (Venkatasubramanian)

University of Toronto (Kim Vicente)

Fore-runner to the **Smart Manufacturing Initiative** (2016)

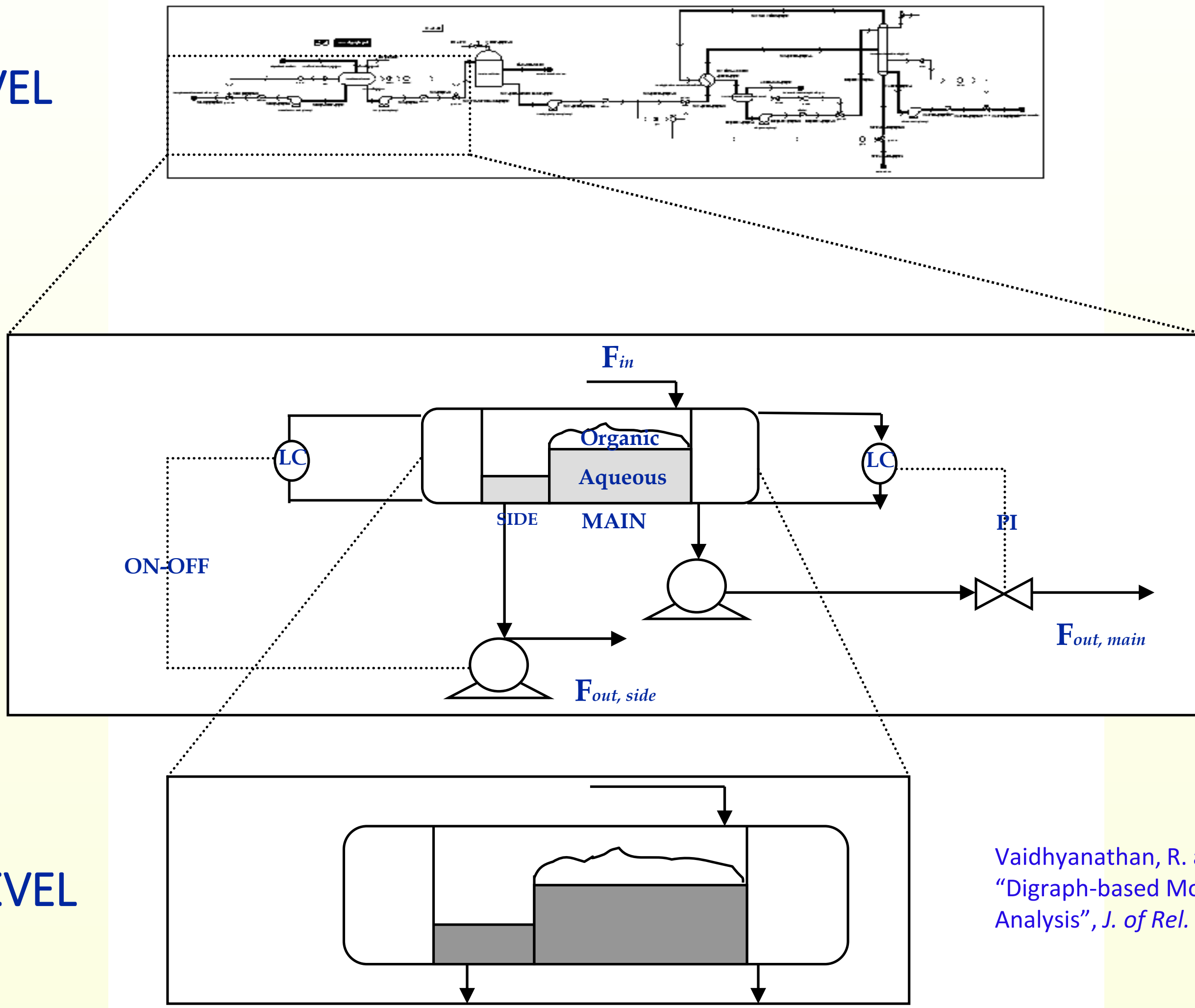
USD $17,000,000 (49% matched back)

Hierarchical Models:
Multi-Scale Causal Modeling Using AI (1995)

PLANT LEVEL

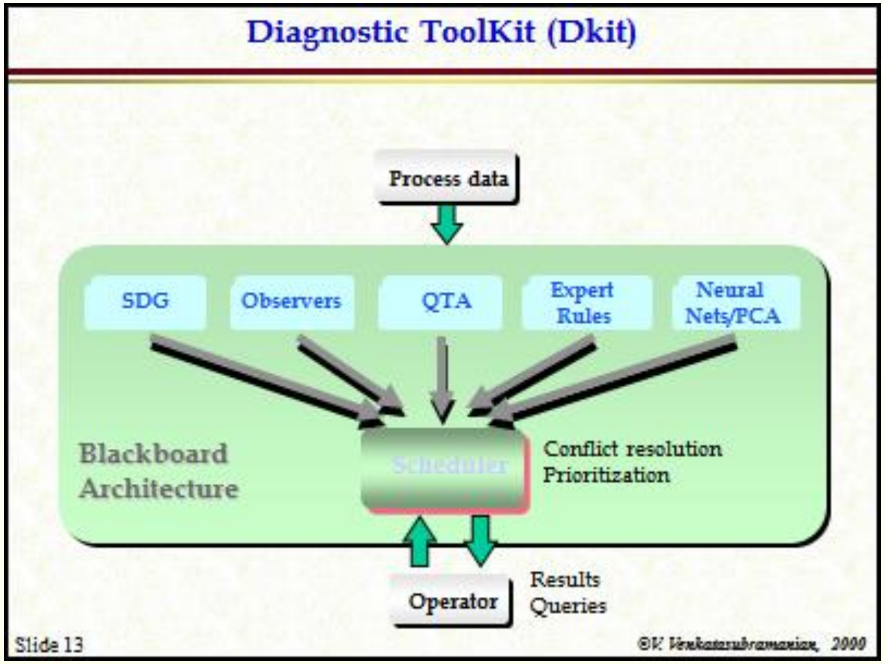
SUBSYSTEM LEVEL

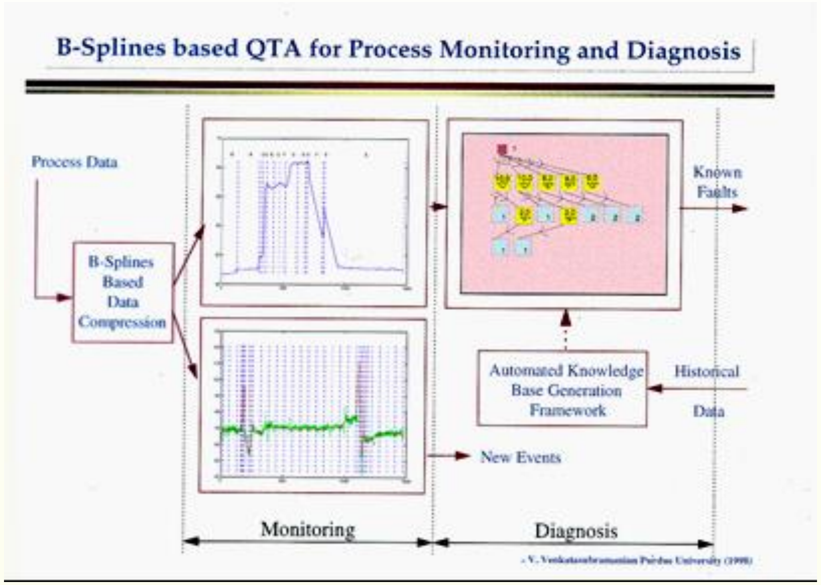
UNIT LEVEL

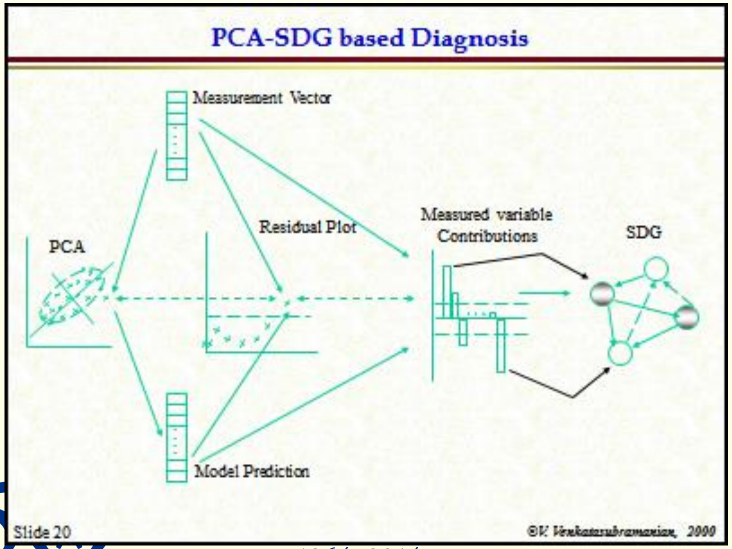


Vaidhyanathan, R. and Venkatasubramanian, V., "Digraph-based Models for Automated HAZOP Analysis", *J. of Rel. Eng. and Sys. Safety*, 50, **1995**.

Intelligent Control System:
Diagnostic ToolKit (DKit, 1993-98)



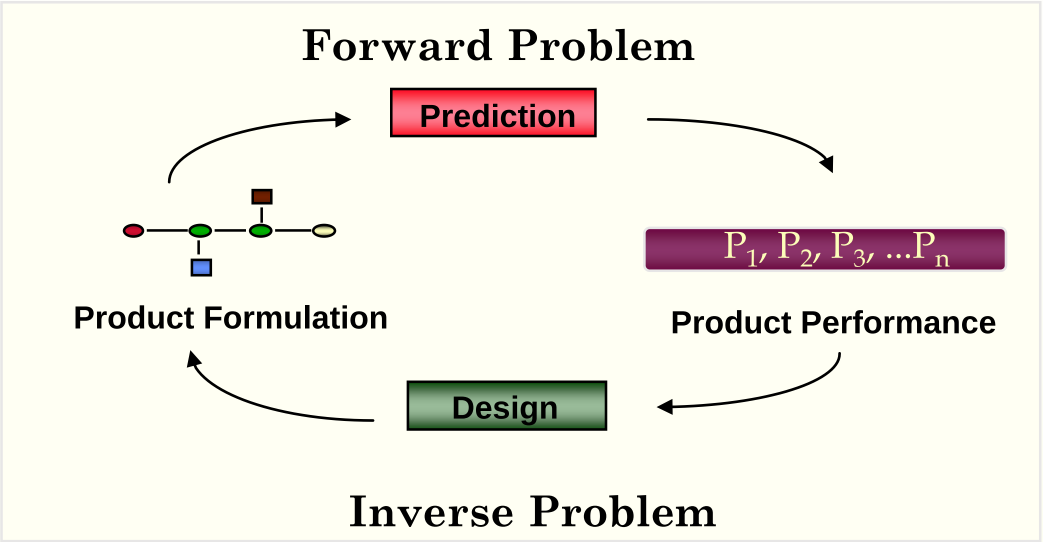




- Implemented in G2, tested at Exxon (Baton Rouge)
- **DKit** successfully diagnosed failures even before the alarms went off (~1/2 – 2 hours ahead)
- **DKit** was licensed to Honeywell in **1998**
- Little impact beyond the prototype: Implementation and Organizational difficulties
- **We were about 20-30 years too early for practical impact!**

Mylaraswamy, Dinkar, *DKit: A Blackboard-based, Distributed, Multi-Expert Environment for Abnormal Situation Management*, Purdue University, PhD Thesis, **1996**.

Inverse Design of Materials (1988-2000): Directed Evolution *in silico*



- Forward Problem
  - Prediction of Performance
  - First Principles + Neural Nets
- Inverse Problem
  - Prediction of Structure or Composition
  - Genetic Algorithm (Directed Evolution *in silico*)

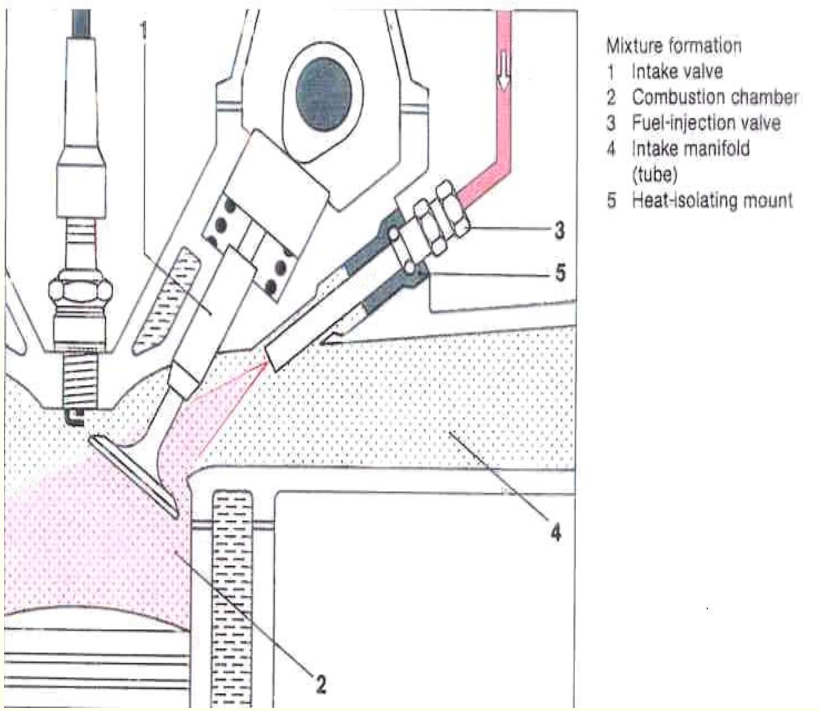
Venkatasubramanian, V., Chan, K. and Caruthers, J.M., "Computer-aided Molecular Design Using Genetic Algorithms", *Computers and Chemical Engineering*, 18 (9), **1994**.

"Genetics cut and paste process can engineer new molecules", *The Dallas Morning News*, October 23, **1995**.

- Frances Arnold (Caltech)
- Directed Evolution *in vitro*
- *Awarded* the Nobel Prize in Chemistry in 2018

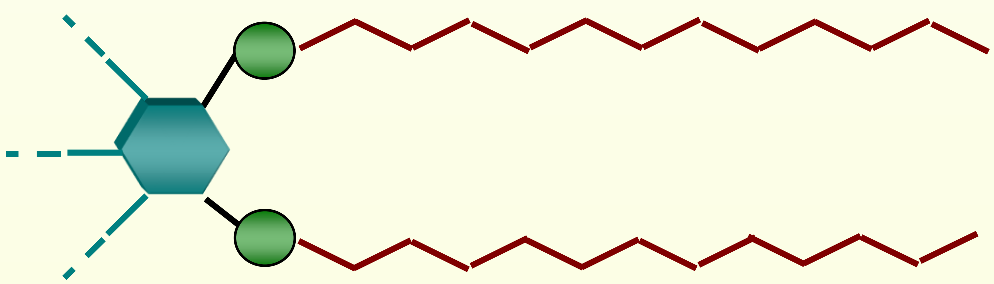
- Fuel Additives (Lubrizol, 1995-99)
- Rubber Compounds (Caterpillar, 1998-2000)

Fuel Additive Design - Lubrizol (1995-2000)

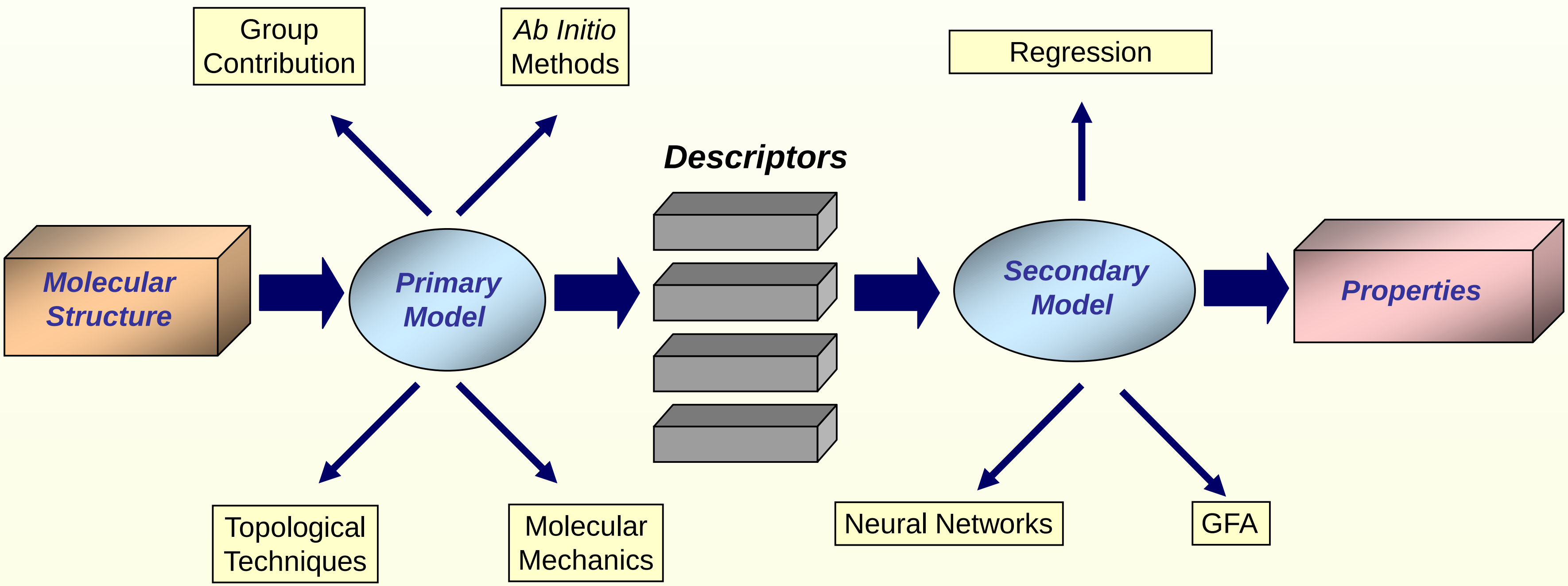


Intake Valve and Manifold

- **EPA Performance Measure**
  - BMW Test for Intake Valve Deposit (IVD)
  - Stipulated to be <100 mg over a 10,000 mile road test
- **Fuel additives are added to gasoline to minimize IVD**
- **Expensive testing**
  - Around $10K for a single datum
- **Not a big data problem**



Hybrid AI Model:
First-Principles + Data Science

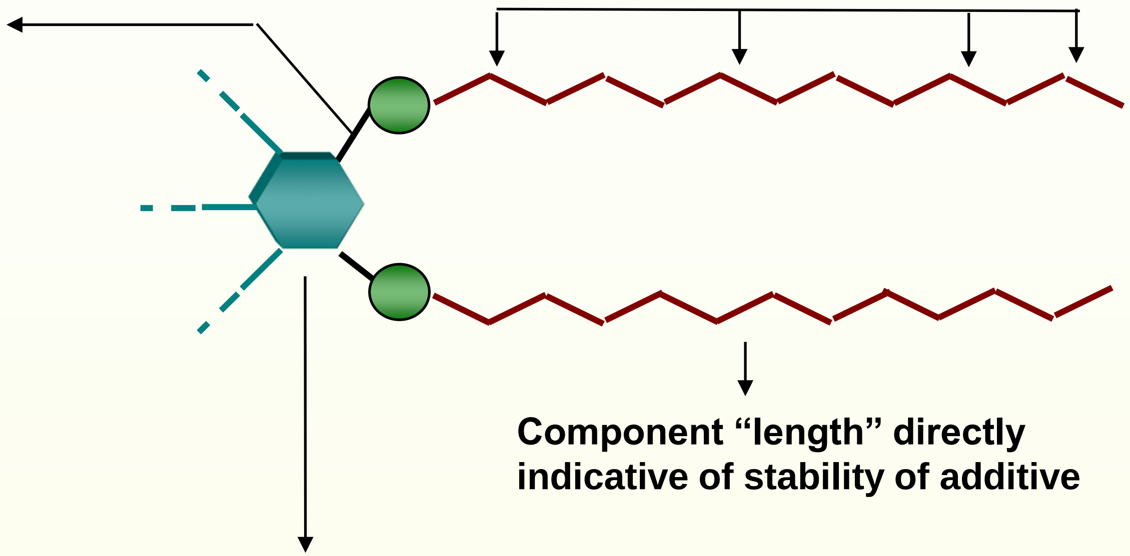


- Sundaram, A., Ghosh, P., and Venkatasubramanian, V., "GENESYS: A Framework for Designer Guided Evolutionary Search for High Performance Products", *Comput. and Chem. Eng*., 23, **1999**.
- Sundaram, A., Ghosh, P., Caruthers, J.M. and Venkatasubramanian, V., "Design of Fuel Additives Using Neural Networks and Evolutionary Algorithms", *AIChE J.*, 47, **2001.**

First-Principles-based Math Model for Additive Degradation

Breakage of this bond removes “dirt” carrying capacity totally

Breaking of these bonds control “length”



Component “length” directly indicative of stability of additive

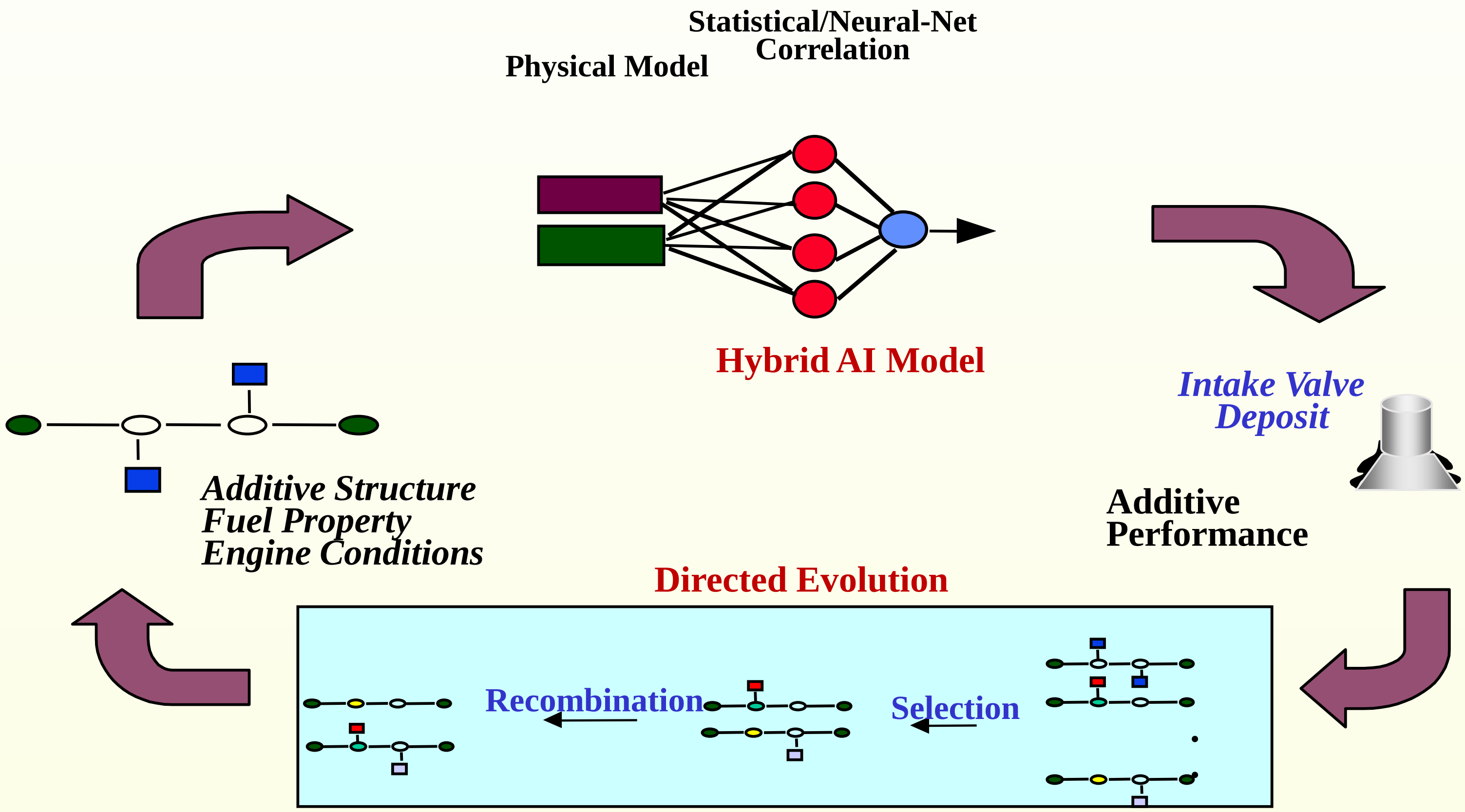
Chemical nature of this component (polar/non-polar) controls “dirt” removing capacity

First-principles-based math model tracks the structural distribution of fuel-additive with time due to reactive degradation

Inverse Design of Materials: Hybrid AI Model

Directed Evolution *in silico* (1995-2001)

Fuel Additives (Lubrizol, 1995-99); Rubber Compounds (Caterpillar, 1998-2001)

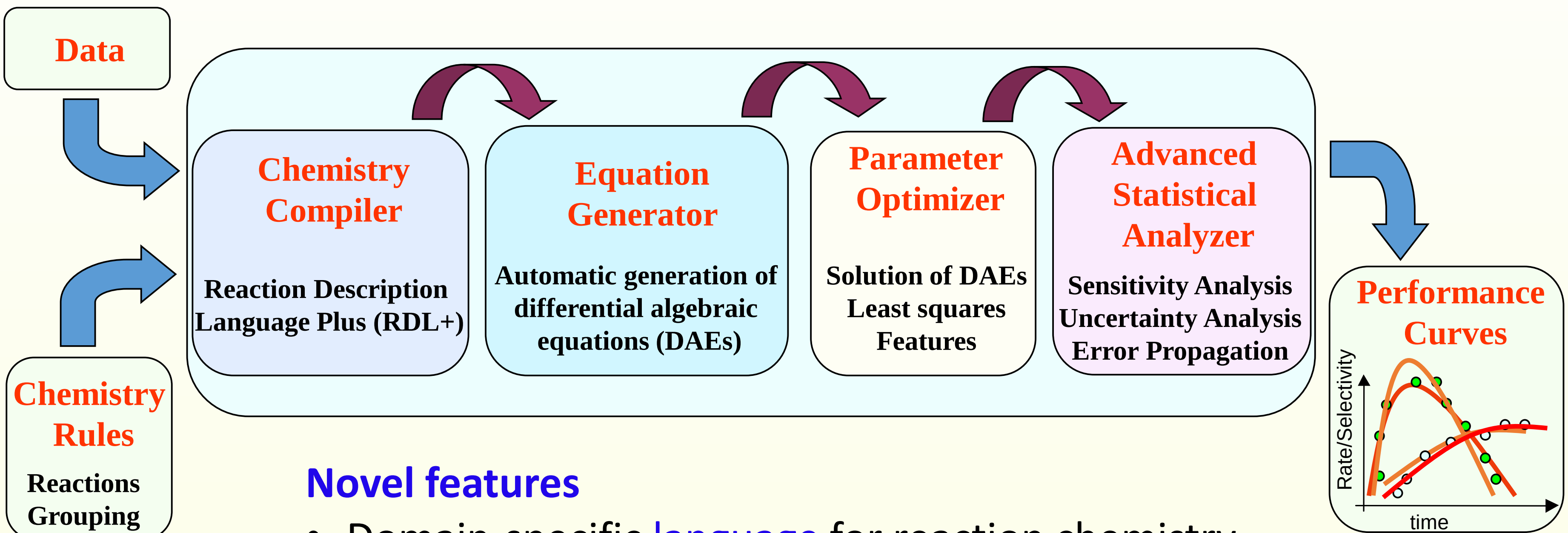


- Sundaram, A., Ghosh, P., and Venkatasubramanian, V., "GENESYS: A Framework for Designer Guided Evolutionary Search for High Performance Products", *Comput. and Chem. Eng*., 23, **1999**.
- Sundaram, A., Ghosh, P., Caruthers, J.M. and Venkatasubramanian, V., "Design of Fuel Additives Using Neural Networks and Evolutionary Algorithms", *AICHE J*., 47, **2001.**

Reaction Modeling Suite:

AI-based Modeling Platform for Catalyst Development (2002-05)

ExxonMobil



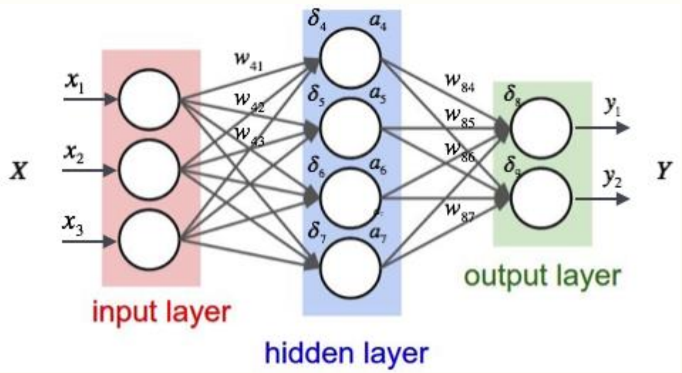
Novel features

- Domain-specific language for reaction chemistry
- Domain-specific compiler
- Chemistry Ontology
- Active Learning

Katare, S., Caruthers, J.M., Delgass, W.N., and Venkatasubramanian, V., "An Intelligent System for Reaction Kinetic Modeling and Catalyst Design", *Ind. Eng. Chem. Res. and Dev.*, 43(14), **2004**.

AI in PSE: Phase II

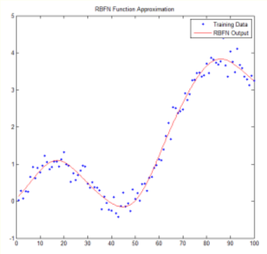
- **Machine Learning I - Neural Networks (~1990 – ~2005)**

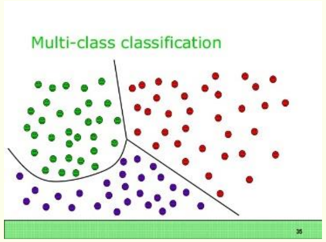


Expert Systems Drawbacks

- Too much time, effort, and specialized expertise
- Did not scale well for industrial applications
- Backpropagation algorithm (1986)
- Bottom-up strategy
- Automatically learned patterns between input and output vectors by adapting the weights

Nonlinear Function Approximation and Classification Problems





Source:
https://medium.com/@curiously/tensorflow-for-hackers-part-iv-neural-network-from-scratch-1a4f504dfa8
https://neustan.wordpress.com/2015/09/05/neural-networks-vs-svm-where-when-and-above-all-why/
http://mccormickml.com/2015/08/26/rbfn-tutorial-part-ii-function-approximation/

Most applications in ChE were in process control and fault diagnosis with some industrial applications

AI Applications in ChE
(1983 – 2010)

- Process monitoring and fault diagnosis
- Process control
- Process design
- Process synthesis
- Process safety analysis
- Optimization
- Planning
- Scheduling
- Materials design

- Prototypes demonstrated in all these areas
- Even some industrial applications fielded
- > 3000 Papers

So, why was AI not impactful in ChE during (1983- 2010)?

- Researchers made great progress on conceptual issues
  - Showed how to formulate and solve these challenging problems
- But we were greatly limited by implementational and organizational difficulties for practical impact
  - Lack of computational power and computational storage
  - Lack of communication infrastructure – No Internet, Wireless
  - Lack of convenient software environment
  - Lack of specialized hardware – e.g., NVIDIA GPU for simulations
  - Lack of data
  - Lack of acceptance of computer generated advice
  - Costs were prohibitive
- Took too much effort, time, and money to field industrial applications
- Doing AI was just too damn hard in those years!
- We were too early, by about 20-30 years!

What is Different Now?

- **Cray-2 Supercomputer (1985)**
  - 1.9 GFLOPS
  - 244 MHz
  - 150 KW!
  - $32 Million! (2010 dollars)
- **Apple Watch (2015)**
  - 3 GFLOPS
  - 1 GHz
  - 1 W!
  - $300!

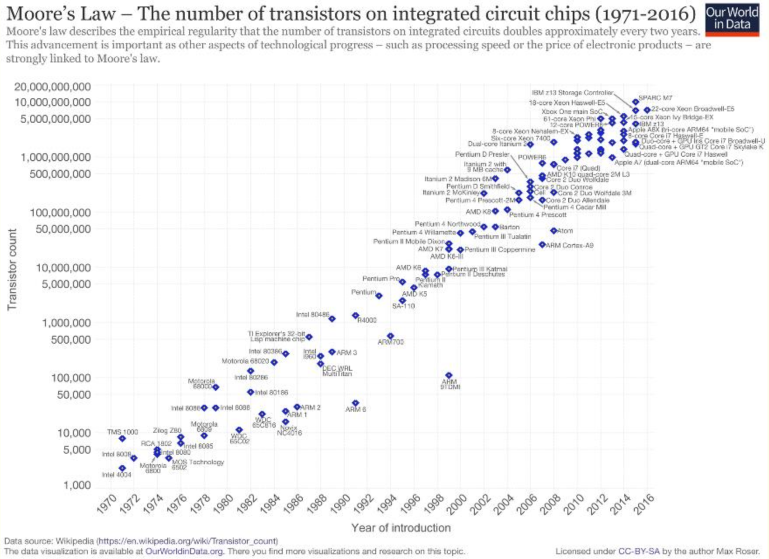
- Performance/unit cost Gain ~150,000x

How Did this Happen?

- Basically Moore's Law happened over the last ~50 years!

Gordon Moore

- All these metrics improved by orders of magnitude!
    - Computational power
    - Computational storage
    - Communication infrastructure: Internet, Wireless
    - Convenient software infrastructure – Python, Java, OWL, …
    - Specialized hardware – graphics processors (GPUs)
    - Big Data
    - Trust & Acceptance – Google, Yelp, Trip Advisor, Tinder, …

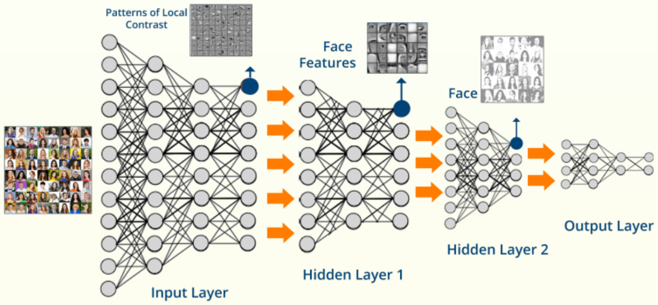


Source: Wiki

- It has become a lot easier and cheaper to develop AI-based solutions

AI in ChE:
Entered Phase III (2005-?)

- **Phase III: Machine Learning II - Data Science (2005 – Present)**
  - Convolution or Deep Nets
  - Reinforcement Learning
  - Statistical Machine Learning
- Hierarchical feature extraction



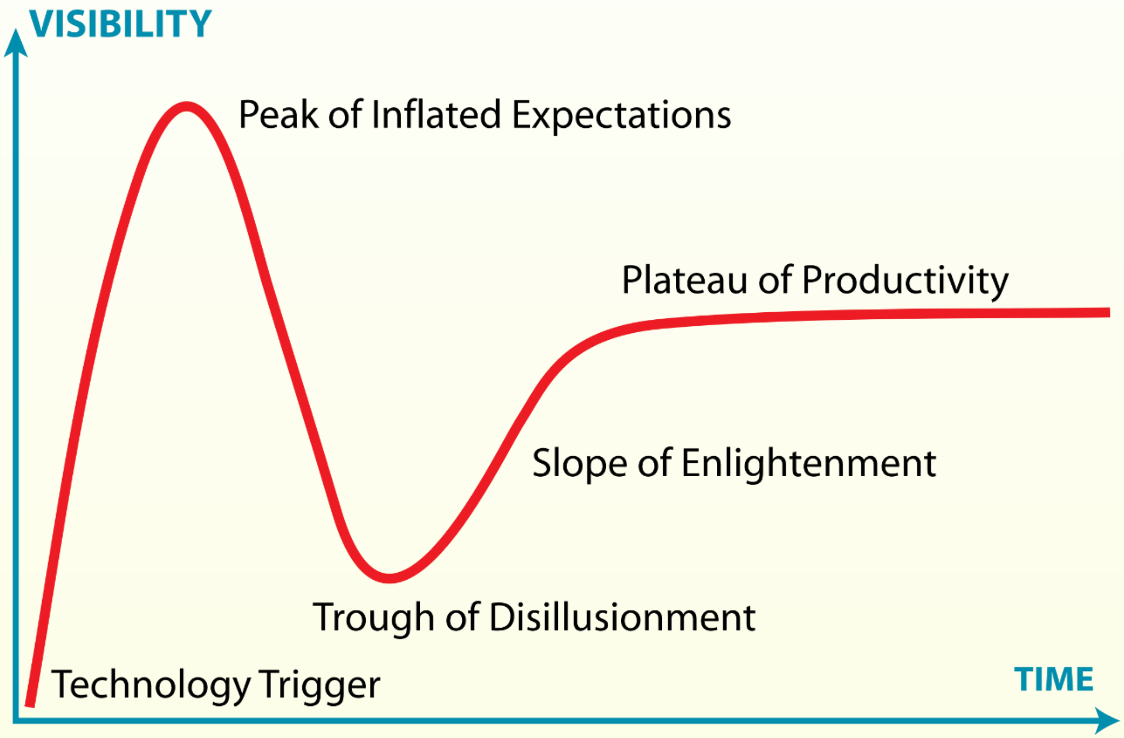
Source: https://cdn.edureka.co/blog/wp-content/uploads/2017/05/Deep-Neural-Network-What-is-Deep-Learning-Edureka.png

- Important ideas, but not really new!
- What really is new are Data, GPU, and Software
- Big impact on NLP, Robotics, Vision
  - Watson, Siri, Alexa, AlphaGo, Self-driving cars

Going Forward:

Challenges and Opportunties

Gartner Hype Cycle



Source: Wiki

Expert Systems: 1980s

Neural Nets: 1990s

Data Science & ML: Now

Data Science and Machine Learning:
Hype vs Reality

- First of all, there is a lot of reinventing the wheel going on
- Many of the "new" techniques are really old ideas from 20-30 years back
    - "Look, Ma, No Hands" self-driving car project at CMU
    - Minivan steered itself for 2,800 of the 2,850 miles between Pittsburgh and San Diego in July 1995
    - Convolutional neural networks are from 1990
    - Autoencoder neural networks are from 1991
    - Inverse design of materials using directed evolution is from 1992
    - Causal models and Explicable AI date from the early 1990s
    - Hybrid models combining first-principles with data-driven techniques are from 1995

https://www.cmu.edu/news/stories/archives/2015/july/look-ma-no-hands.html

- It's worth reading the old papers!

Data Science and Machine Learning: Hype vs Reality

- One doesn't necessarily need convolutional networks, reinforcement learning, etc., for many problems in ChE
  - Other simpler and more transparent AI techniques are often adequate
- ChE or Materials Science problems are often not Big Data!
  - Our domain is different from game playing, vision, and speech
- How do we leverage the prior knowledge that we already have about our materials, processes, and systems?

Lack of Mechanistic Understanding

- Does a self-driving car "know" and "understand" the concepts of momentum, acceleration, force, and Newton's laws, as we do?
- Its behavior is like that of a cheetah chasing an antelope in the wild
- Both display great mastery of the dynamics of the chase, but do they "understand" these concepts?
- Current AI systems have animal-like mastery of their tasks, but they have not gained deeper "understanding" as humans do
- Mechanistic causal understanding is important in many ChE applications such as diagnosis, control, and safety to build credibility
- Cost of mistakes in ChE can be quite high compared to recommendation systems like Yelp, Rotten Tomatoes, …

Source: Wiki

Conceptual Challenges and Opportunities: "Easy" Problems

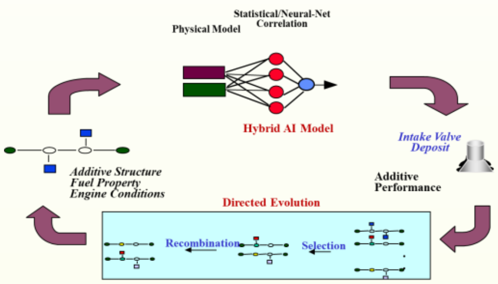
- Large amounts of Data + Easy to use ML tools

- Many recent industrial applications in this category
  - Oil-well performance
  - Wind turbines monitoring
  - Yield improvement, …
  - Estimating physical properties from structures/compositions
  - Determination of structural features
  - Nanoparticle packing, …

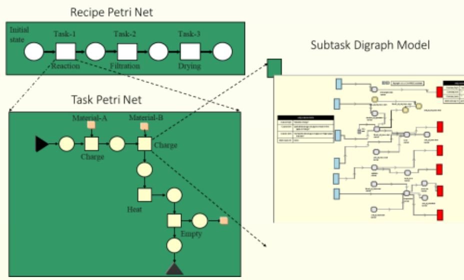
- Lots of recent industrial applications of this category

Conceptual Challenges and Opportunities: "Hard" Problems

- Hybrid AI Models
  - First-Principles + Data-driven
  - Building Physics and Chemistry into Data-driven models



- Causal models
  - Building cause-and-effect relationships for generating explanations and insights
  - Signed Digraph (SDG) Models

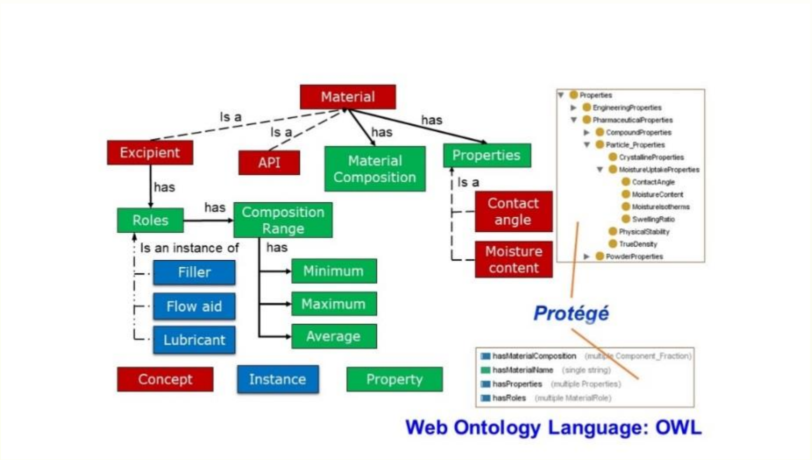


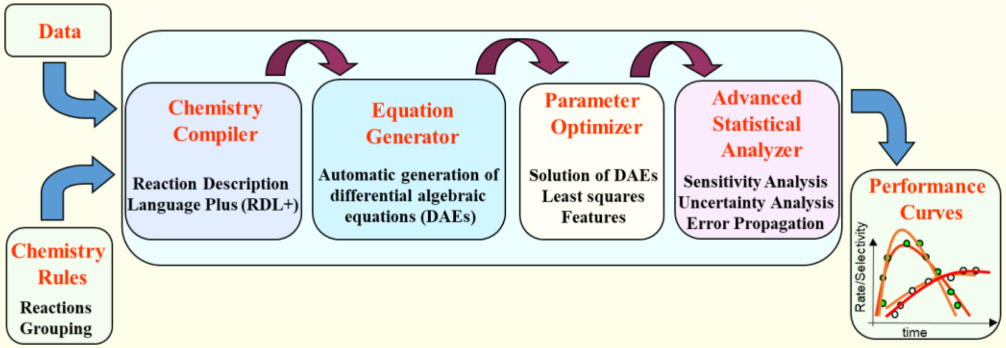
- Combining Symbolic and Numeric AI

- Will take ~10 years to do easily, systematically, and correctly

Conceptual Challenges and Opportunities: "Harder" Problems

- "Watson"-like systems
- Domain-specific
  - Ontologies
  - Languages
  - Compilers …
- Will take ~10-20 years





How about
Conceptually "Hardest" Problems?

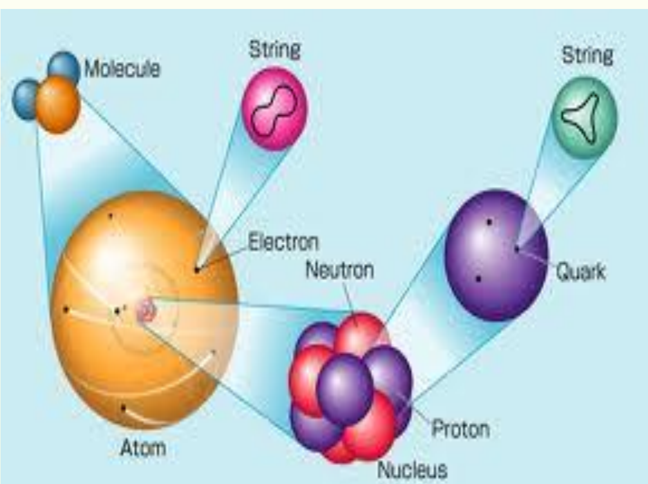
- Phase I: Expert Systems (1983-2000)
- Phase II: Neural Nets (1990-2005)
- Phase III: Data Science (2005 - ?)
- Phase IV: Self-organizing Intelligent Systems (Present?)

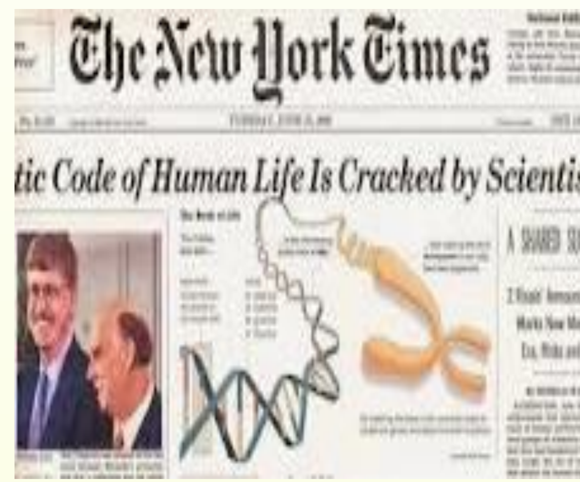
AI: Phase IV (Present?)

- Most intellectually exciting and challenging problem!
- Science of Self-organizing Intelligent Systems
- Modeling, predicting, and controlling the behavior a large population of self-organizing intelligent agents
  - Drone swarms, Robots, Self-assembling nanostructures, Neurons, ..
- Design, Control, and Optimization through Self-organization
- Brand new Science of Emergence
- Grand conceptual challenges here

Science of Self-organizing Systems

- **20th Century Science was largely Reductionist**
  - Quantum Mechanics and Elementary Particle Physics
  - Molecular Biology, Double Helix, Sequencing Human Genome

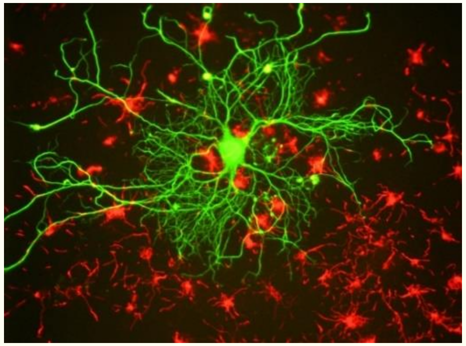



The New York Times

tic Code of Human Life Is Cracked by Scientist

Complex Self-organizing Systems

- But can **reductionism** answer the following question?
- Given the properties of a neuron, can we predict the behavior of a system of 100 billion neurons?



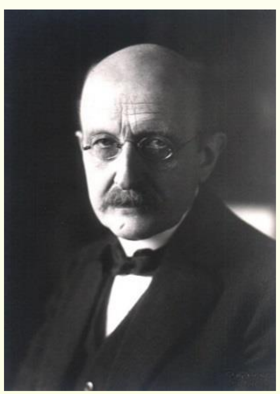
- From **Neuron** → **Brain** → **Mind**
- How do you go from Parts to System?

Reductionism cannot answer this!
There is nothing left to "reduce"!

Two Small Clouds at the Dawn of 20th Century

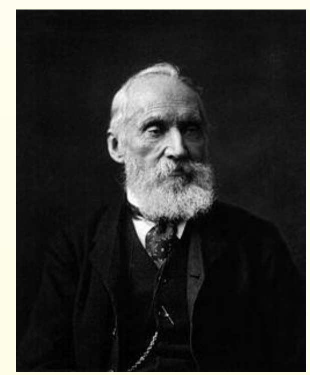
- Lord Kelvin's lecture, Royal Society, London, in April 1900
- "Nineteenth Century Clouds Over the Dynamic Theory of Heat and Light"
- "Physics knowledge is almost complete, except for two small "clouds" that remain over the horizon"
- These small "clouds" Revolutionized 20th Century Physics
  - Blackbody Radiation: Quantum Mechanics
  - Michelson-Morley Null Experiment: Relativity

Max Planck



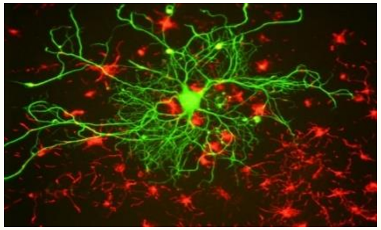
Albert Einstein

Lord Kelvin



"Large Cloud" at the Dawn of 21st Century

- How do you go from **Parts to Whole**?



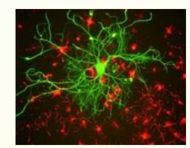
- Need an **Constructionist** Theory of **Emergent Behavior**
- Requires a new conceptual synthesis across AI, Systems Engineering, Statistical Mechanics, Game Theory, and Biology
- What might such a theory look like?
- I have been pursuing this since 1983

Theory of Parts-to-System

- Individual agent properties → Emergent properties of millions of agents

- Agents are "dumb" (molecules) → System (gas)
  - Statistical Thermodynamics

- What if the agents are "intelligent"?
  - e.g., neurons, robots, or people
- Can we generalize statistical thermodynamics?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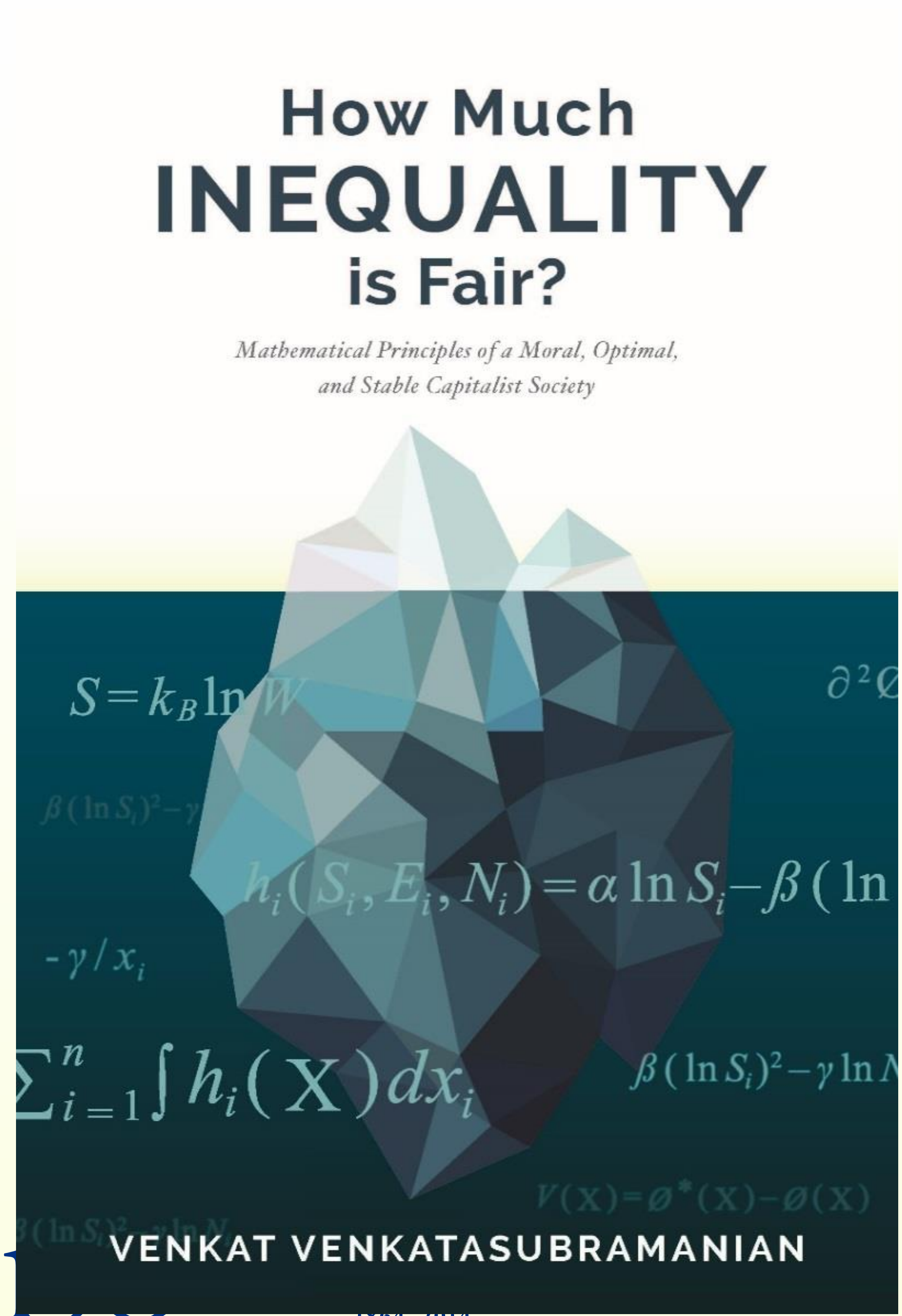
- Statistical Thermodynamics ("Dumb" agents) $\xrightarrow{\text{34 years}}$ Statistical Teleodynamics ("Intelligent" agents)

- Telos means goal in Greek



- Mathematical and Conceptual Foundations of Statistical Teleodynamics
- Theory of Parts-to-System in Economics
- Constructionist Theory of Emergence of Income Distribution
- 200-year-old open question
- Conceptual synthesis of
  - Political Philosophy
  - Economics
  - Game Theory
  - Statistical Mechanics
  - Information Theory
  - Systems Engineering

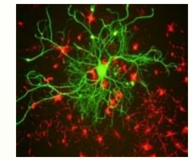
Columbia University Press
Economics Series
July 2017

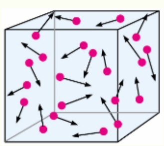
1864–2014

CRIS.lab

Mathematical Theory of Emergence

- How do you go from Neuron to Brain to Mind?
- How about Statistical Teleodynamics for the Brain?
- What is the Mathematical Theory of Consciousness?
- Most important scientific question of the 21st Century



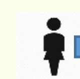



"Semi-rational" agents: Neurons
Cognitive Neuroscience

"Dumb" agents: Molecules
Thermodynamics

"Intelligent" agents
"Perfectly Rational" people
Neoclassical Economics

- Requires a new conceptual synthesis across
  - AI
  - Systems Engineering
  - Information Theory
  - Statistical Mechanics
  - Game Theory
  - Cognitive Neuroscience



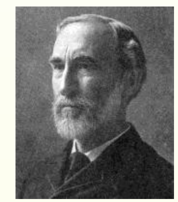

V. Venkatasubramanian, "Statistical Teleodynamics: Toward a Theory of Emergence", *Langmuir*, 33 (42), pp. 11703–11718, 2017.

Challenges and Opportunities

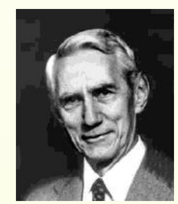
- Theory of Emergence: Parts-to-Whole
  - How do you Design, Control, and Optimize via Self-Organization?
  - Revolutionize Economics, Neuroscience, Political Philosophy, Climate Change, …
  - Key is Entropy


Carnot
(1796-1832)

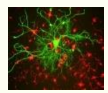

Clausius
(1822-1888)


Gibbs
(1839-1903)


Boltzmann
(1844-1906)


Shannon
(1916-2001)

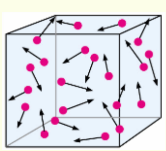

Jaynes
(1922-1998)




Cognitive System
Entropy??

Consciousness?

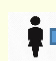
Thermodynamic System
Entropy is Disorder

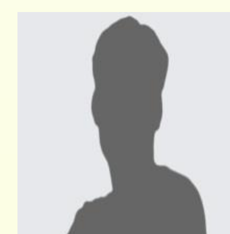


34 yrs

Socio-Economic System
Entropy is Fairness

Inequality
Justice

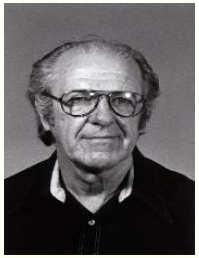


Summary

Knowledge Modeling in ChE: Evolution of Three Paradigms

- **Differential-Algebraic Equations (DAE): Amundson Era (1950s)**
- Modeling Process Units
- Modeling First-principles



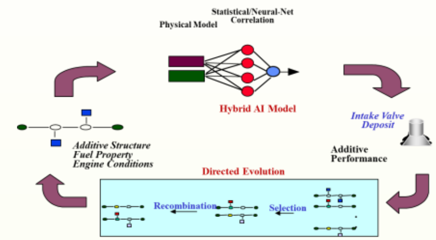
- **Optimization (MILP, MINLP): Sargent Era (1970s)**
- Modeling Process Engineers: Decision-making
- Modeling Constraints

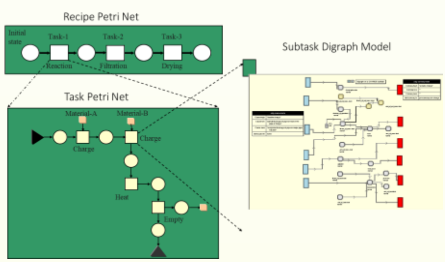
- **Artificial Intelligence Westerberg, Stephanopoulos, and others (1980s)**

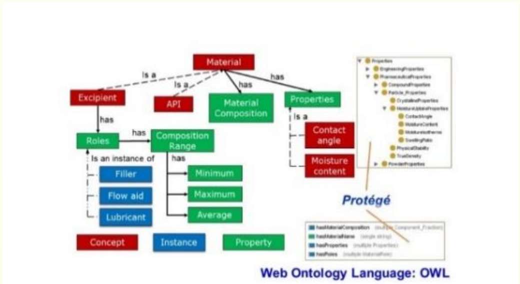
- Modeling Process Engineers & Data: Decision-making
- Modeling Symbolic Structures and Relationships

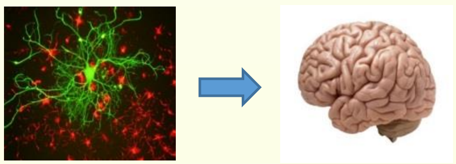
Challenges and Opportunities

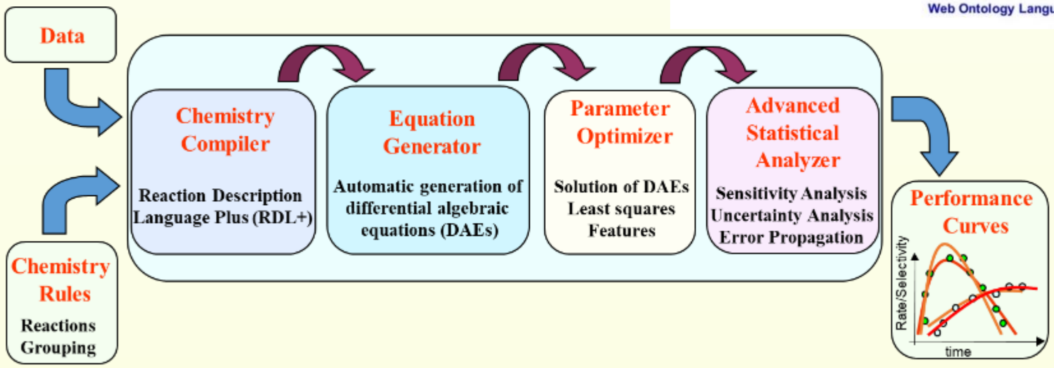
- We need progress on
  - Hybrid AI Models: First-Principles + Data-driven Models
  - Causal modeling
  - Discovery Engines: Domain-specific Ontologies, Languages, Compilers
  - How to combine Symbolic AI with Numeric AI?
- Need to be able to scale such systems quickly, easily, and reliably
- Science of the 21stCentury: Theory of Emergence - From Parts-to-Whole











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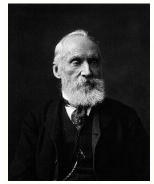


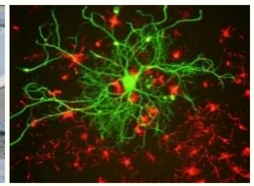



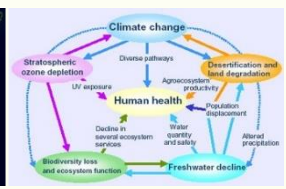

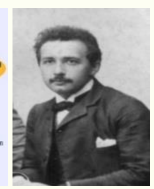

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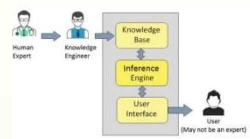
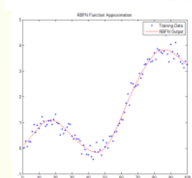
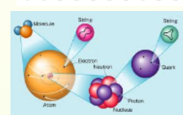


https://www.tutorialspoint.com/artificial_intelligence/artificial_intelligence_expert_systems.htm



http://mccormickml.com/2015/08/26/rbfn-tutorial-part-ii-function-approximation/



http://www.rikenresearch.riken.jp/eng/frontline/4584

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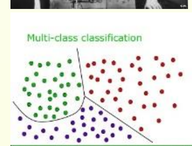
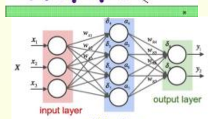


https://neustan.wordpress.com/2015/09/05/neural-networks-vs-svm-where-when-and-above-all-why/



https://medium.com/@curiousily/tensorflow-for-hackers-part-iv-neural-network-from-scratch-1a4f504dfa8

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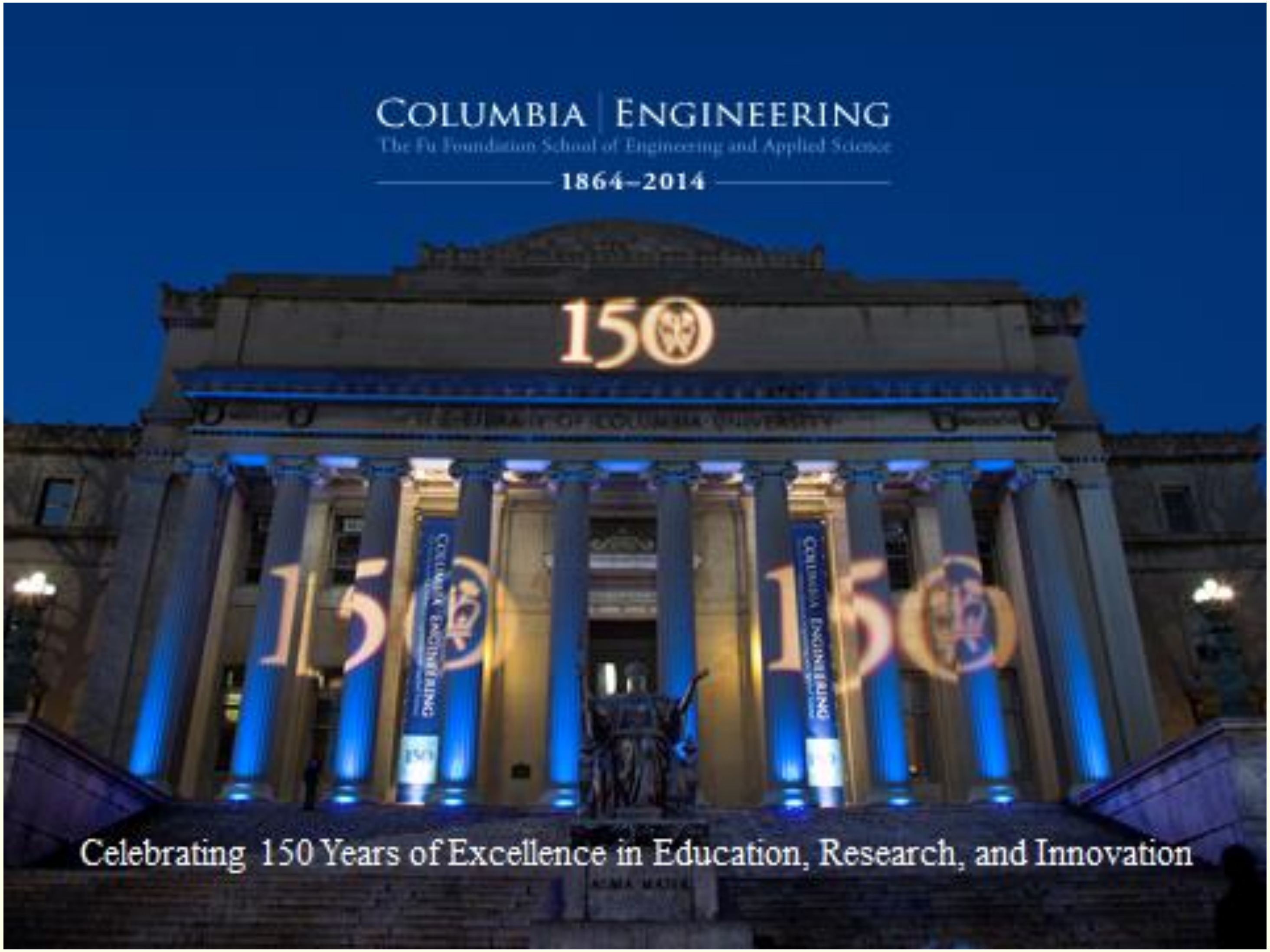

Questions?