2020:
A Perspective on the Horizon Through an Innovation Lens
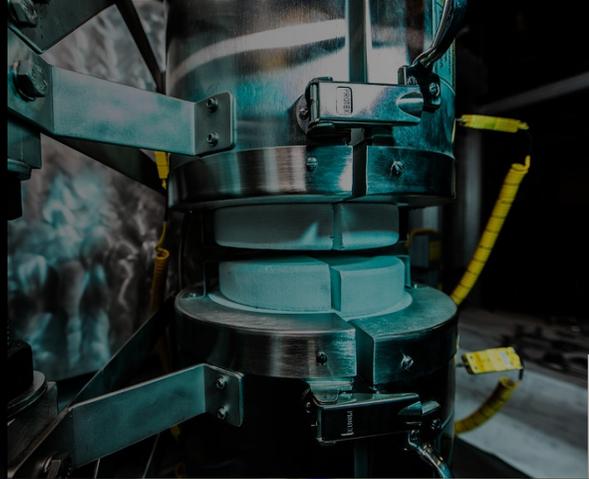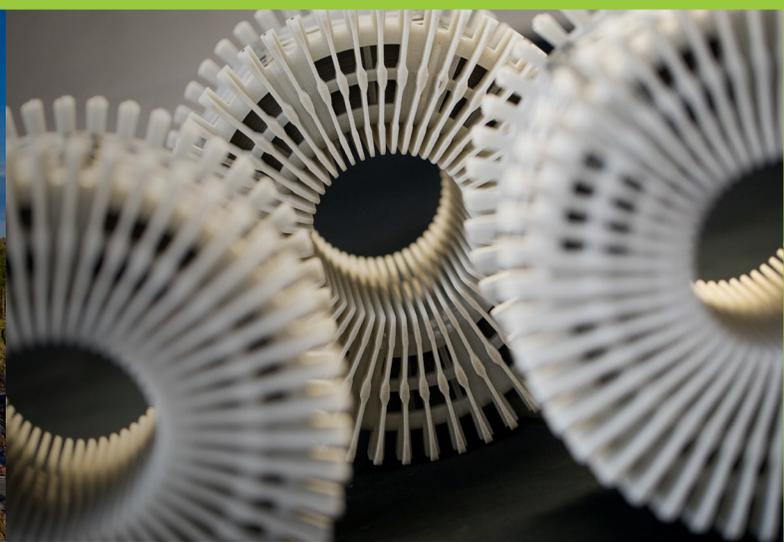September 8, 2020
Randall W. Gentry – NETL CRO

Agenda

1. A perspective on Innovation (an over used term)

2. Why is AI Important to the Story?

3. A nod to Bayes!

4. Why is Coal Important t the Story?

5. The Role of "Integrated Energy Systems"?

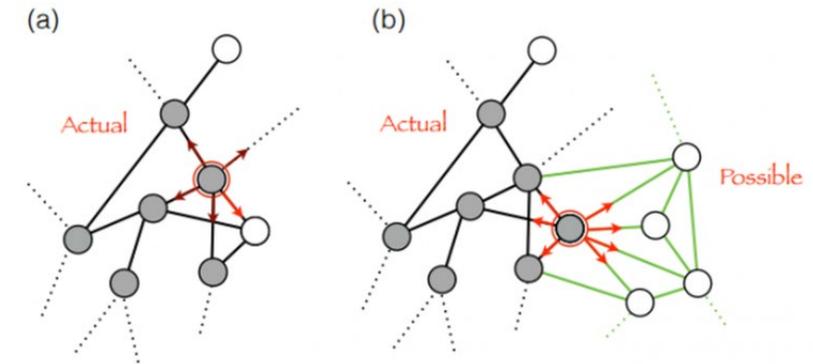6. Questions & Answers

1. A Perspective on Innovation

Artificial Intelligence

Mathematical Model Reveals the Patterns of How Innovations Arise

The work could lead to a new approach to the study of what is possible, and how it follows from what already exists.

by **Emerging Technology from the arXiv**   Jan 13, 2017

Novelties versus Innovation

- New to the individual
- New to the world

"These results provide a starting point for a deeper understanding of the adjacent possible and the different nature of triggering events that are likely to be important in the investigation of biological, linguistic, cultural, and technological evolution."

Manuscript: arXiv:1701.00994v1 [physics.soc-ph] 4 Jan 2017 - Dynamics on expanding spaces: modeling the emergence of novelties

Source: MIT Technology Review January 13, 2017

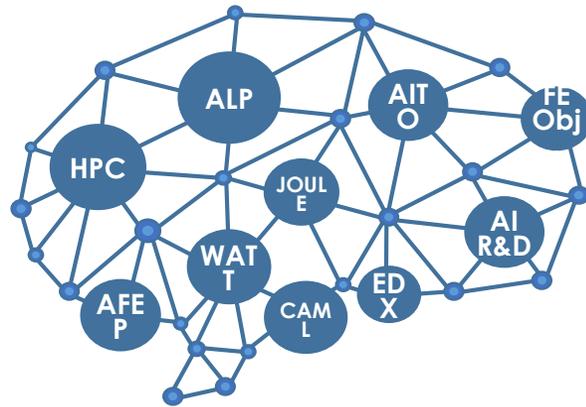Emergent Ideas for future User facilities and Innovation Hubs

Characterization of Materials at New Scales

HPC at new scales with AI Hardware

Large-Data Manipulation and computation "Deep Knowledge extraction"

Facilities

Investments in Research Infrastructure

Albany

**Advanced Alloy
Development Facility**

**Geological Environmental
Science Visualization Center**

Pittsburgh

**Center for Data Analytics
and Machine Learning**

Morgantown

**Sensitive Compartmented
Information Facility**

**Computational Science and
Engineering Center - Joule 3.0**

Example NETL Key Laboratory Initiatives (KLI)

Science-based Artificial Intelligence/Machine Learning Institute (SAMI)

Enables crosscutting applications of science-based AI/ML within the defense, aerospace, automotive, security, health and medical sectors.

Microwave Reaction Chemistry

Significantly improves the energy efficiency of industrial processes, increasing selectivity, and enabling scalable and distributed low carbon applications.

2. Why is AI Important to the Story?
A topic that has been around since 1950s

1952-1956

1990

Google (1998)

2011

Birth of AI

"Gaussian" likelihood because we use a normal distribution

ANN
Intelligent Agents

Big Data
Deep Learning
High Performance Computing

Gaussian Naïve Bayes Classifier

Bayes' theorem

In probability theory and statistics, Bayes' theorem describes the probability of an event, based on prior knowledge of conditions that might be related to the event. Wikipedia

Prior Belief

$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)}$$

A, B = events
$P(A|B)$ = probability of A given B is true
$P(B|A)$ = probability of B given A is true
$P(A), P(B)$ = the independent probabilities of A and B

Posterior Belief

Not calculated in Naïve classifier approaches

Google Brain

Google Brain is a deep learning artificial intelligence research team at Google. Formed in the early 2010s, Google Brain combines open-ended machine learning research with information systems and large-scale computing resources. Wikipedia

Start date: 2011

Location: Mountain View, California

Google Brain
Tensor Flow
Deep Learning
"Tensor Hardware"

3. *A nod to Bayes!*

and perhaps others

Thomas Bayes came to prominence after his death when his friend and colleague Richard Price read his work before the Royal Society 1763. The work which was a problem of inverse probability was presented in "***An Essay towards solving a Problem in the Doctrine of Chances***" which was read to the Royal Society in 1763.

It is no simple fact that without this singular work, much of what exists in the field of AI and ML would not exist today in its current form.

4. Why is Coal important to the Story?

- A rich source for C-C and C-H (aromatic and aliphatic) chemistry which may offer unique new materials pathways into the manufacturing supply chain for 'high value' needed product line (i.e. graphitic or graphene related materials, etc.).

A memristor computer memory device that is enabled by a coal-derived graphene material manufactured at NETL.

A cement sample that is enhanced with a coal-derived graphene material manufactured at NETL.

Coal-derived fluorescent graphene quantum dots that are being evaluated for biosensor and medical diagnostic applications.

5. The role of "Integrated Energy Systems?"

Design and Optimization of Novel Multi-Input, Multioutput Hybrid Energy Systems to Power a Clean Energy Future [*Under Review*]

D. Arent,* S. Bragg-Sitton, D. Miller, T. Tarka, J. Engel-Cox, R. Boardman, P. Balash, M. Ruth, J. Cox, D. J. Garfield
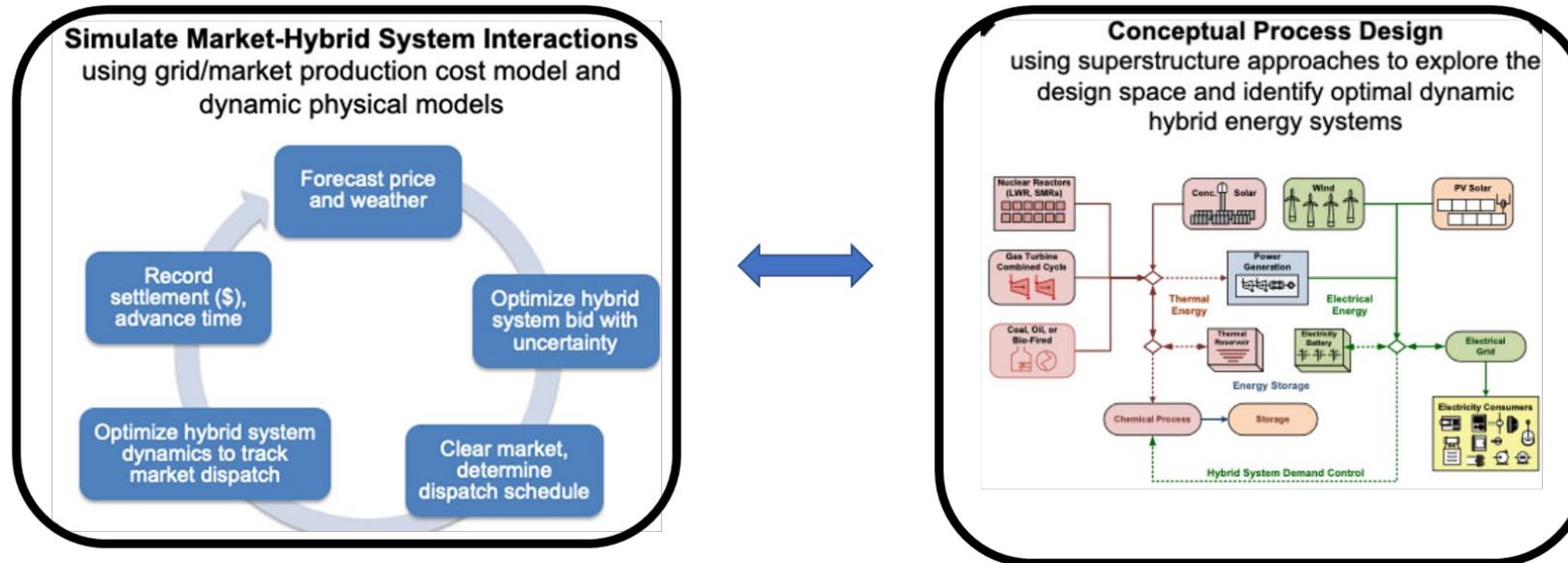
A proposed integration of process and grid/market models and tools that could be leveraged to identify optimal technology solutions on a regional basis.

Q&A