New York Scientific Data Summit 2020:

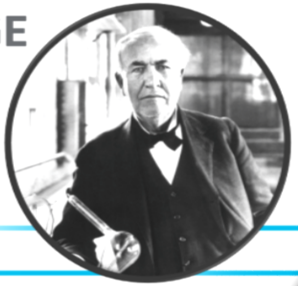
Data-Driven Discovery in Science and Industry

Organized by: BROOKHAVEN NATIONAL LABORATORY, COLUMBIA UNIVERSITY IN THE CITY OF NEW YORK, FLATIRON INSTITUTE, NYU, RUTGERS THE STATE UNIVERSITY OF NEW JERSEY, Stony Brook University, TEXAS The University of Texas at Austin

WEDNESDAY, OCTOBER 21 - CRITICAL INFRASTRUCTURE/MANUFACTURING

Computational Modeling at GE

Richard Arthur
Sr. Principal Engineer, GE Research



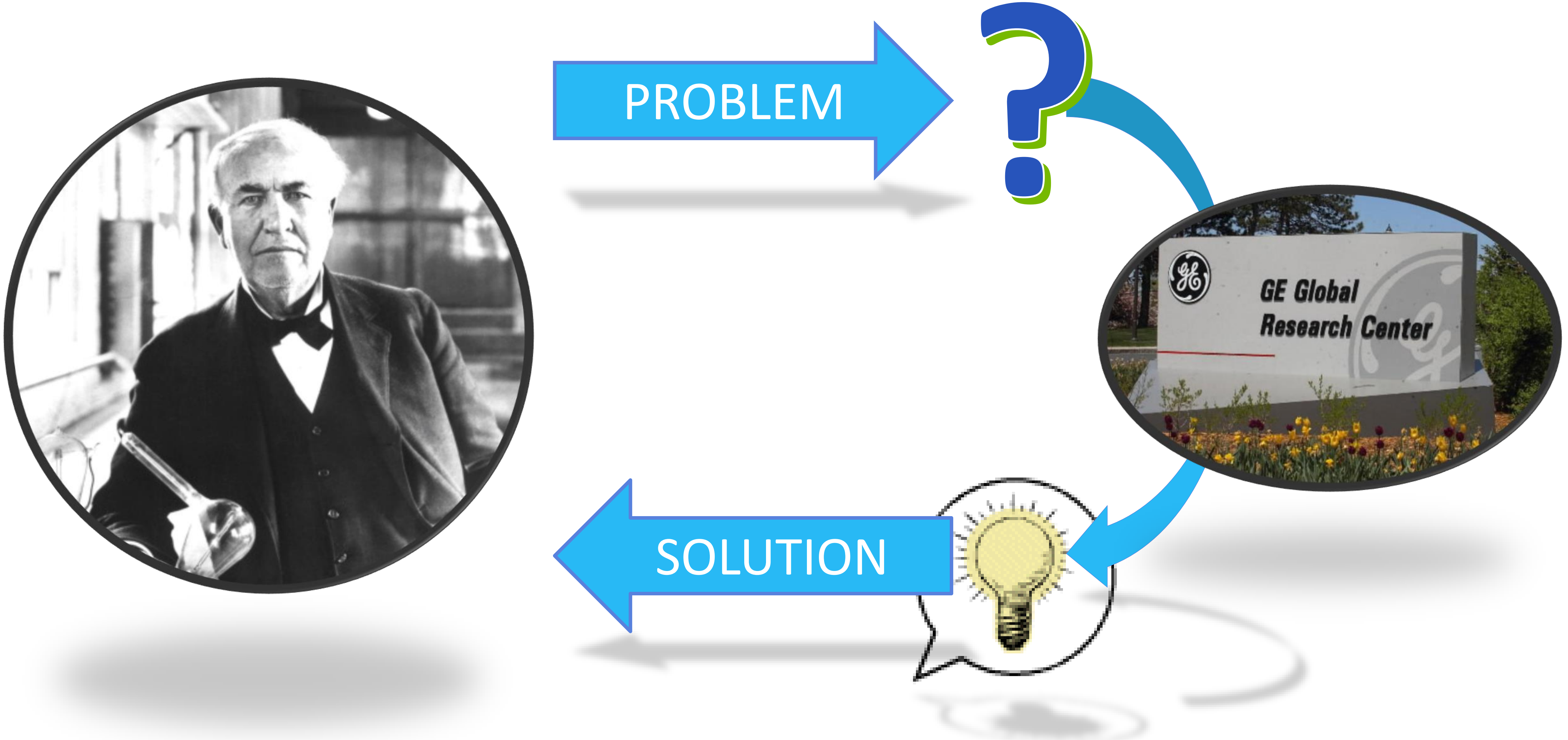
Engineering's core competency is **Problem Solving**

https://blogs.ge.com/problem-solving

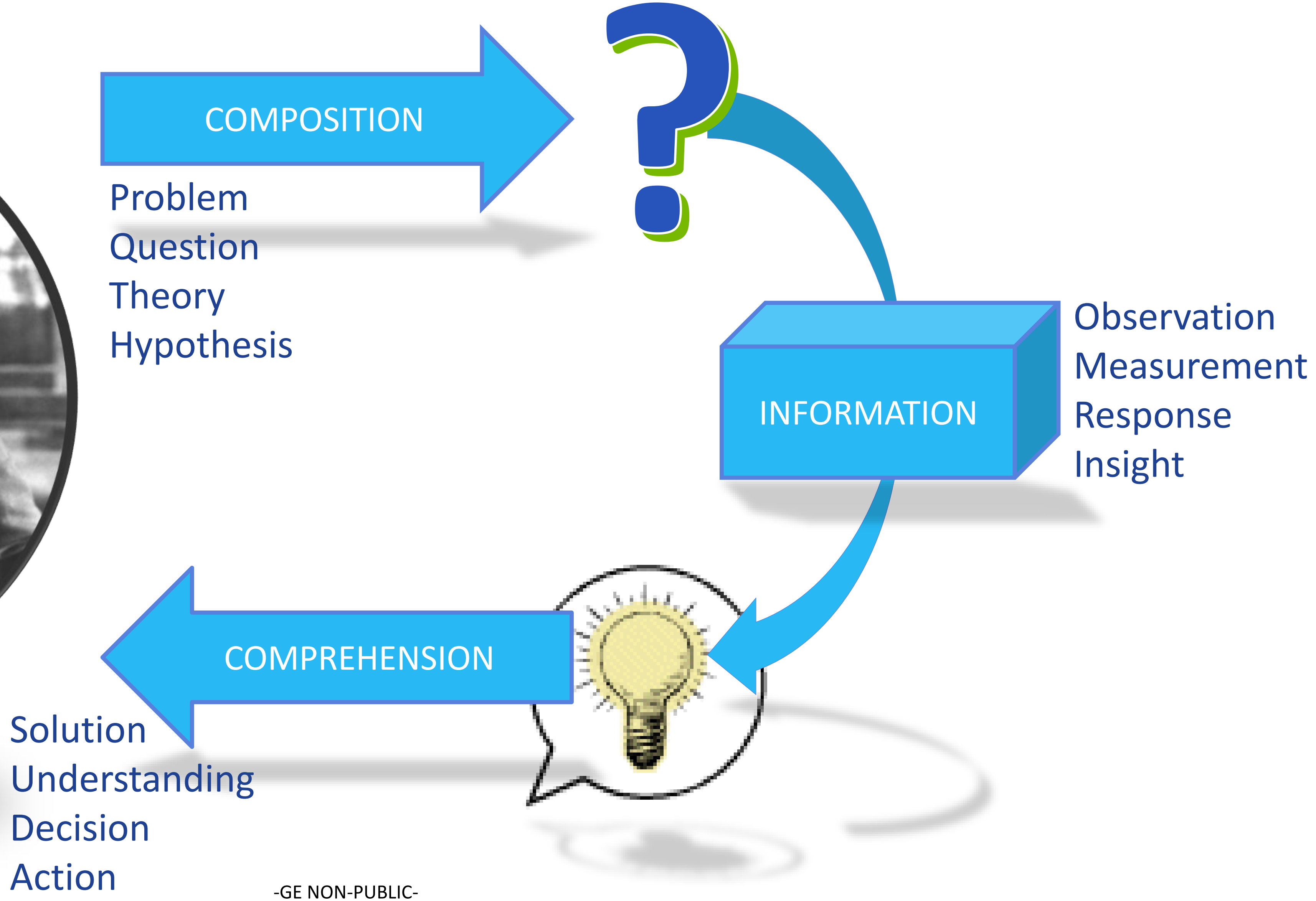
Team,

One of my personal resolutions for 2020 is to teach more about lean as we drive our transformation. I will work to do that more often this year in my emails to you. For today's note I'm starting with problem solving because it is foundational to developing competitive advantage, delivering for our customers and ultimately improving our performance over the long-term.

Problem Solving is Engineering’s Core Competency



Problem Solving



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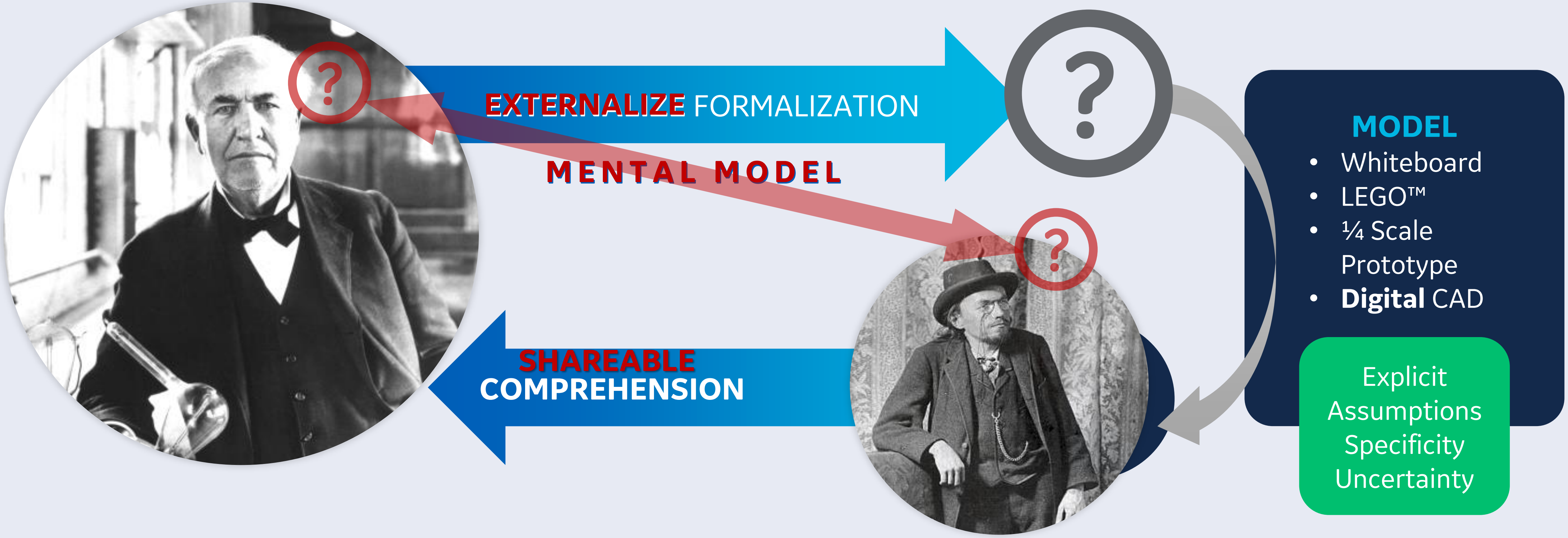
Problem Solving** critically relies upon **Modeling
(the problem, the solution and the process in between)

All decisions and actions employ models



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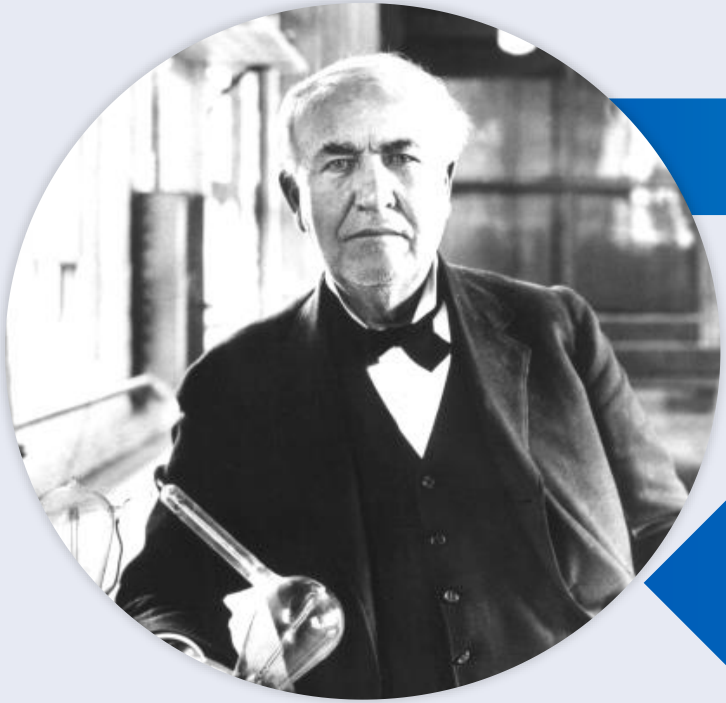


COMPOSE PROBLEM

Inform & Advise Decision/Action
Answer Question
Explain Observation
Insight Discovery

COMPREHEND SOLUTION

Problem Modeled
Mapped Decision Space
Trade-off Analysis

MODEL

- Traceability
- Reproducibility
- Verification & Validation
- Confidence Bounds
- Assumptions, Unknowns & Sources of Error

Scientific method

THEORY

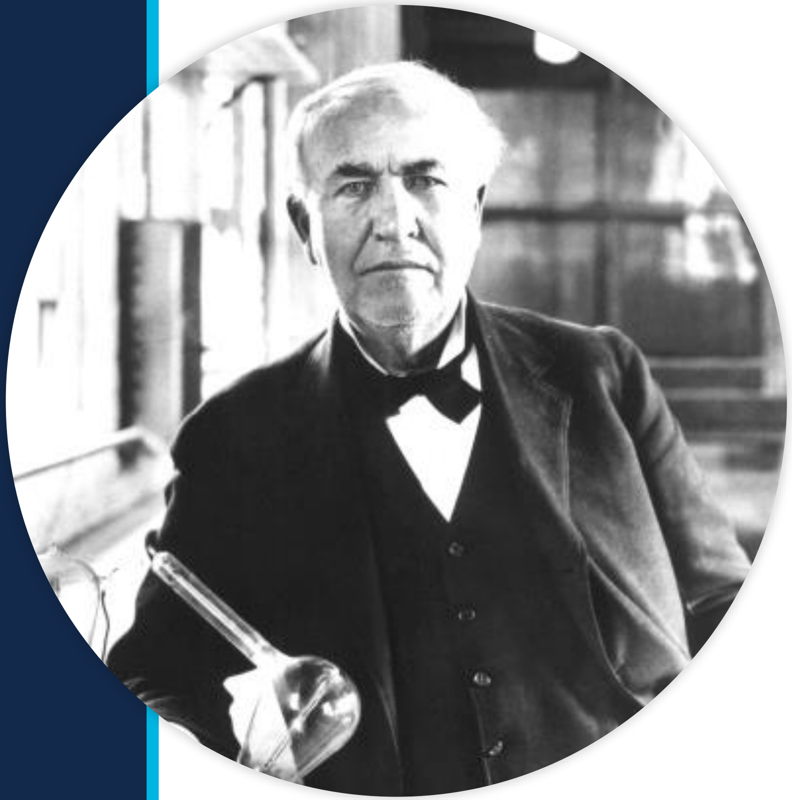
TEST

Math

Experimentation

THEORETICAL
MODEL

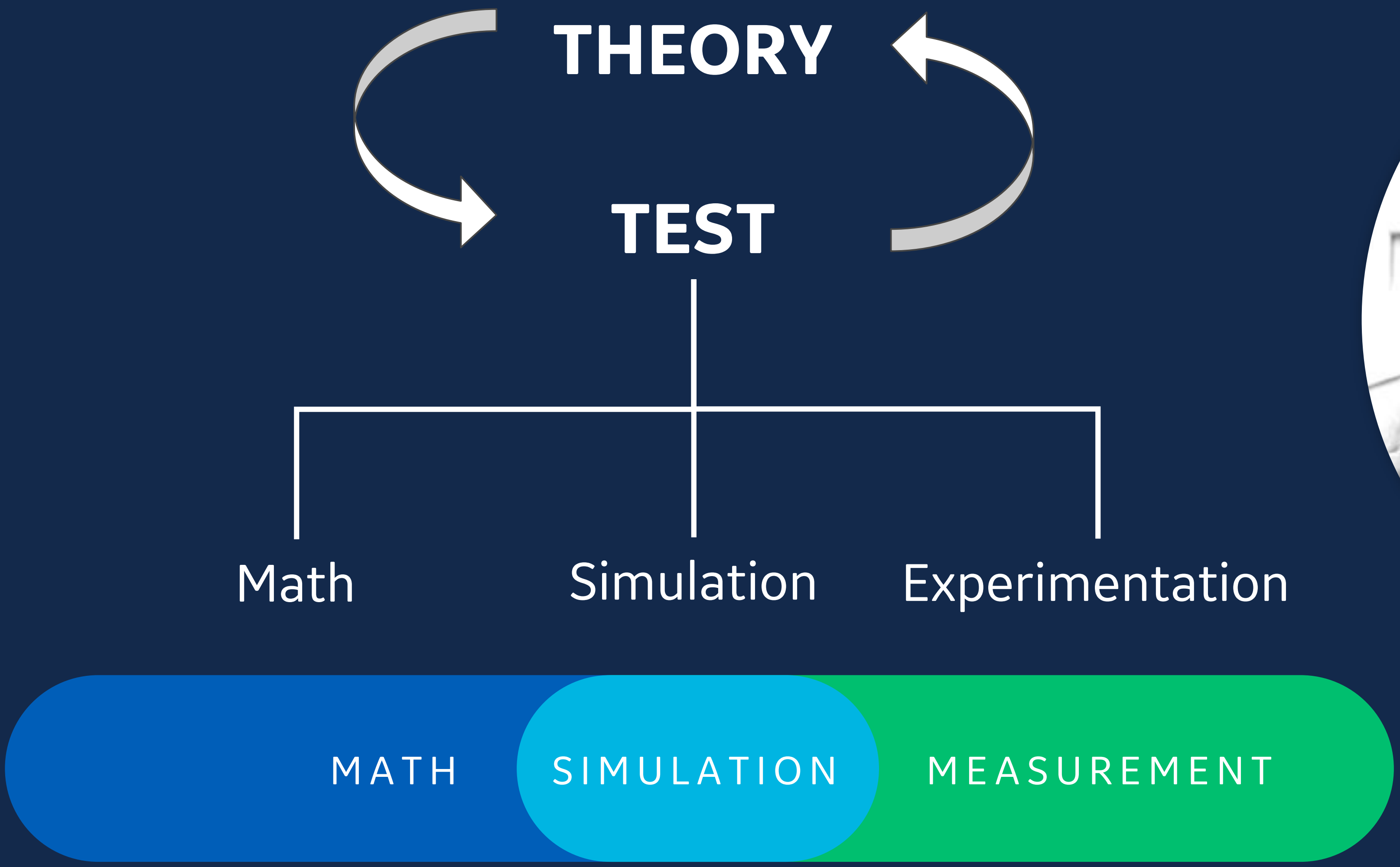
EMPIRICAL
EXPERIMENTAL
OBSERVATION

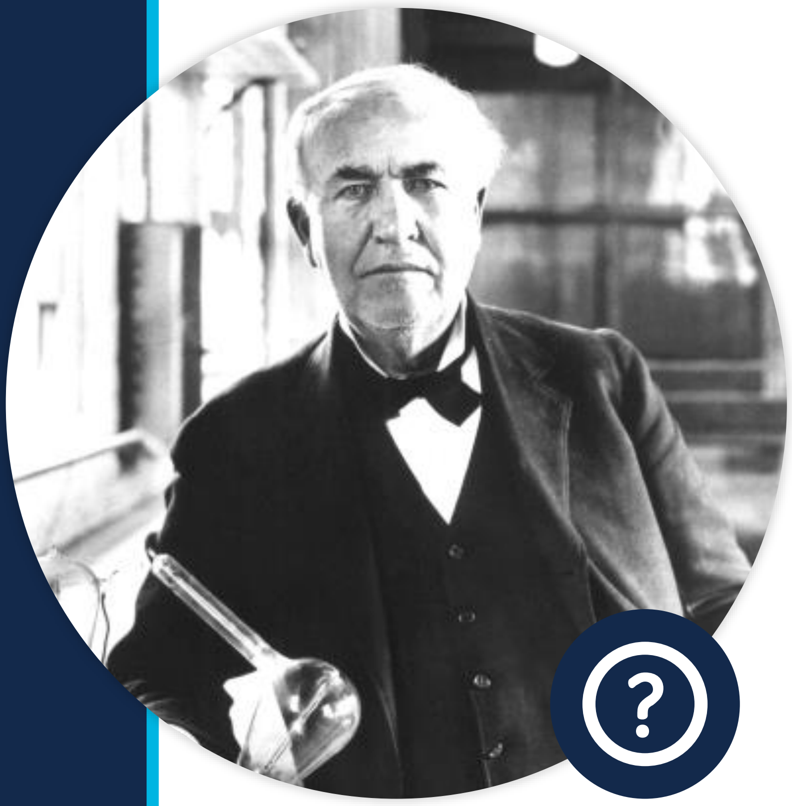


EDISONIAN

$$$$ Testing & Measurement

Modern practice of scientific method





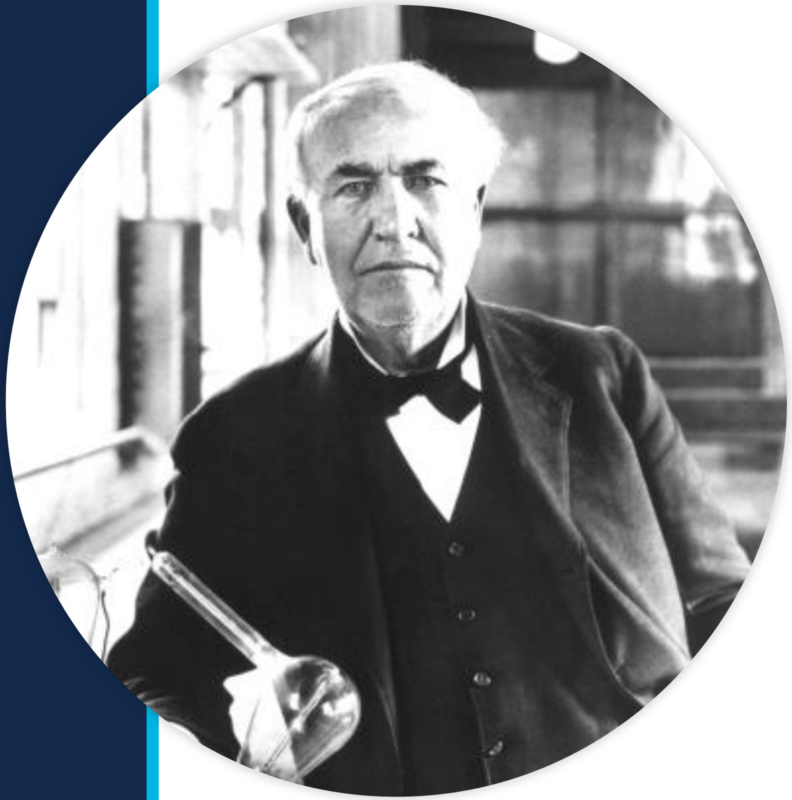
Advancing the Scientific Method

DESIGN

TEST

- Theory
- Simulation
  - Bypass physical limitations
  - Synthetic universal properties
  - Only “digital waste”
- Experiment

THEORY | SIMULATION | EXPERIMENT **$100’s of MM** PER YEAR AT GE



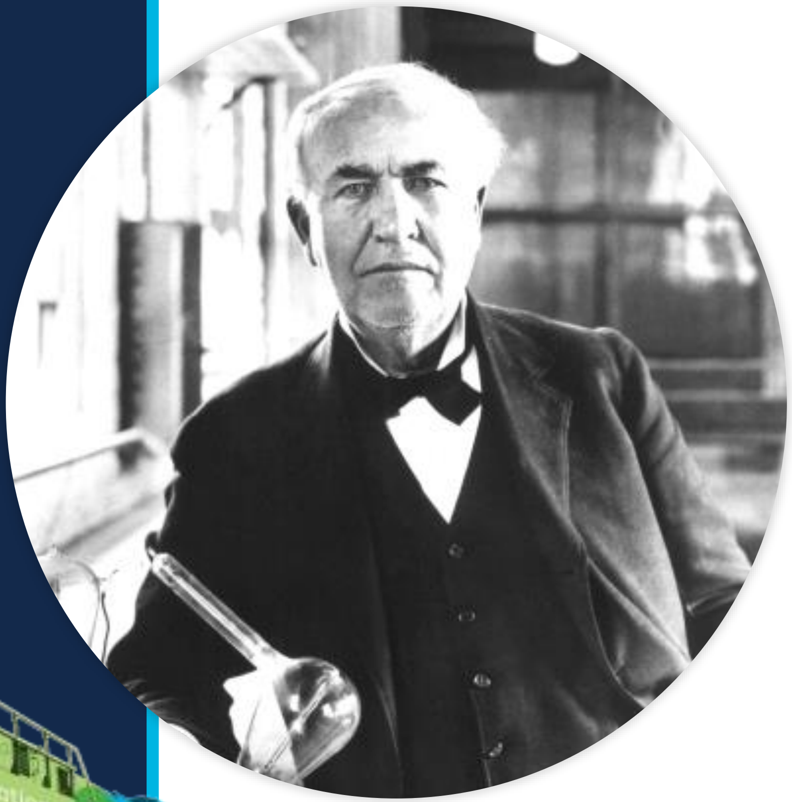
COMPUTATIONAL MODEL? I’M SKEPTICAL!

CRITICAL INFRASTRUCTURE

DESIGN

TEST

Justified Model Skepticism: Garbage IN/Garbage OUT

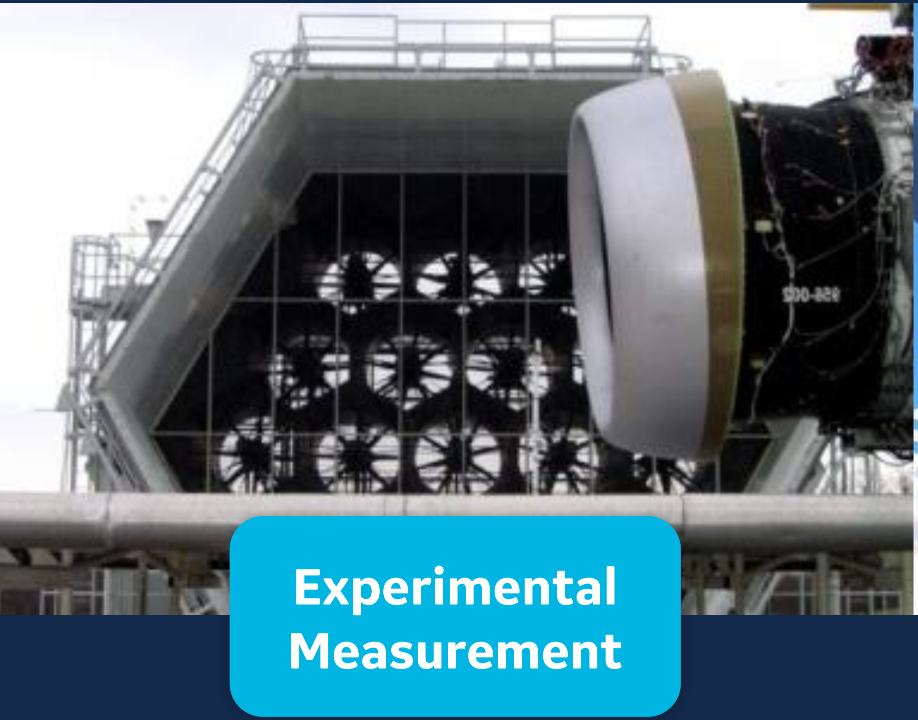


GE Legacy Products:

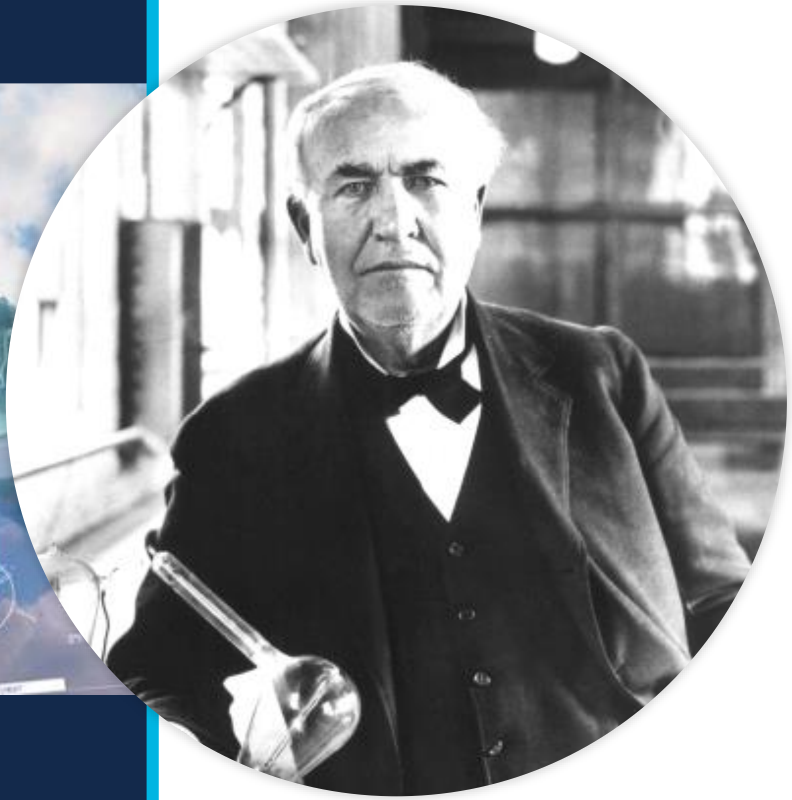
- are Highly Complex &
- High Value Assets,
- have Safety-Critical Components,
- High-Consequence Downtime,
- and Long Field Life

Physical validation is critical

“RIG” TEST



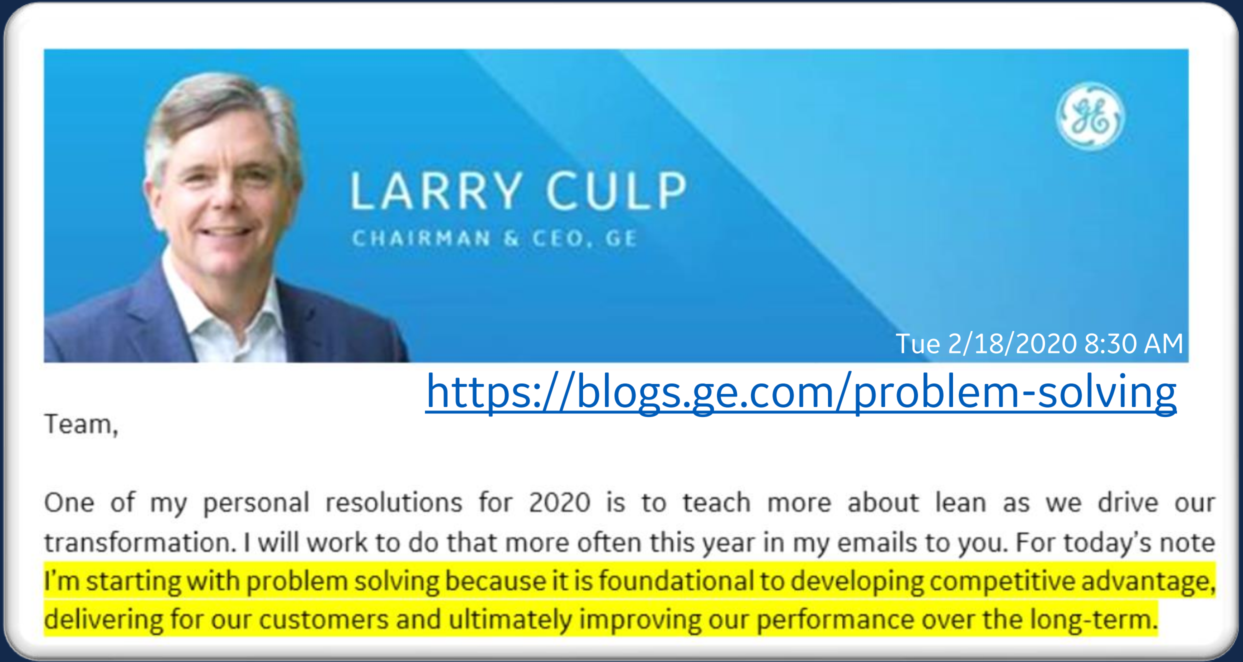
DIGITAL TWIN



VERIFICATION & VALIDATION

CALIBRATION & UNCERTAINTY QUANTIFICATION

Engineering's core competency is **Problem Solving**



LARRY CULP

CHAIRMAN & CEO, GE

Tue 2/18/2020 8:30 AM

https://blogs.ge.com/problem-solving

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Problem Solving *critically relies upon* ***Modeling***
(the problem, the solution and the process in between)

Modeling *critically relies upon* ***Computational Methods***
(as an engine for scale, productivity, consistency and capability)

Computational model as scientific instrument



MICROSCOPE

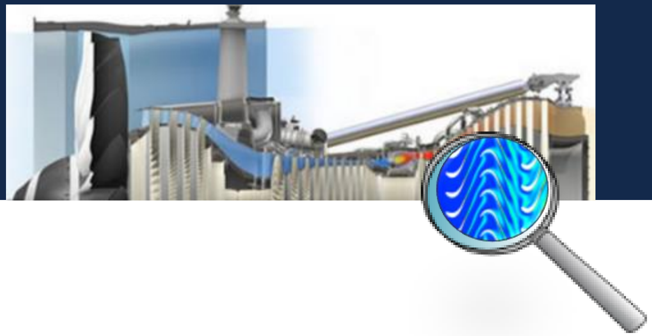
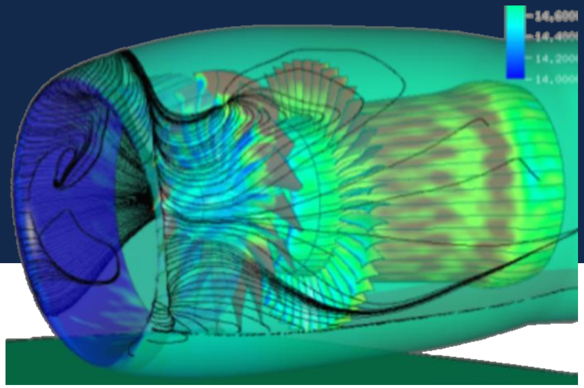
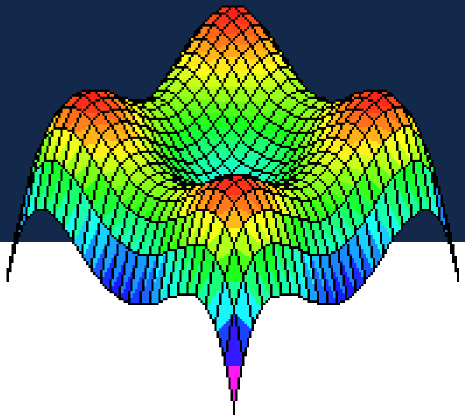
Interrogate extreme detail

MACROSCOPE

Perceive system-wide interactions

CAMPAIGN

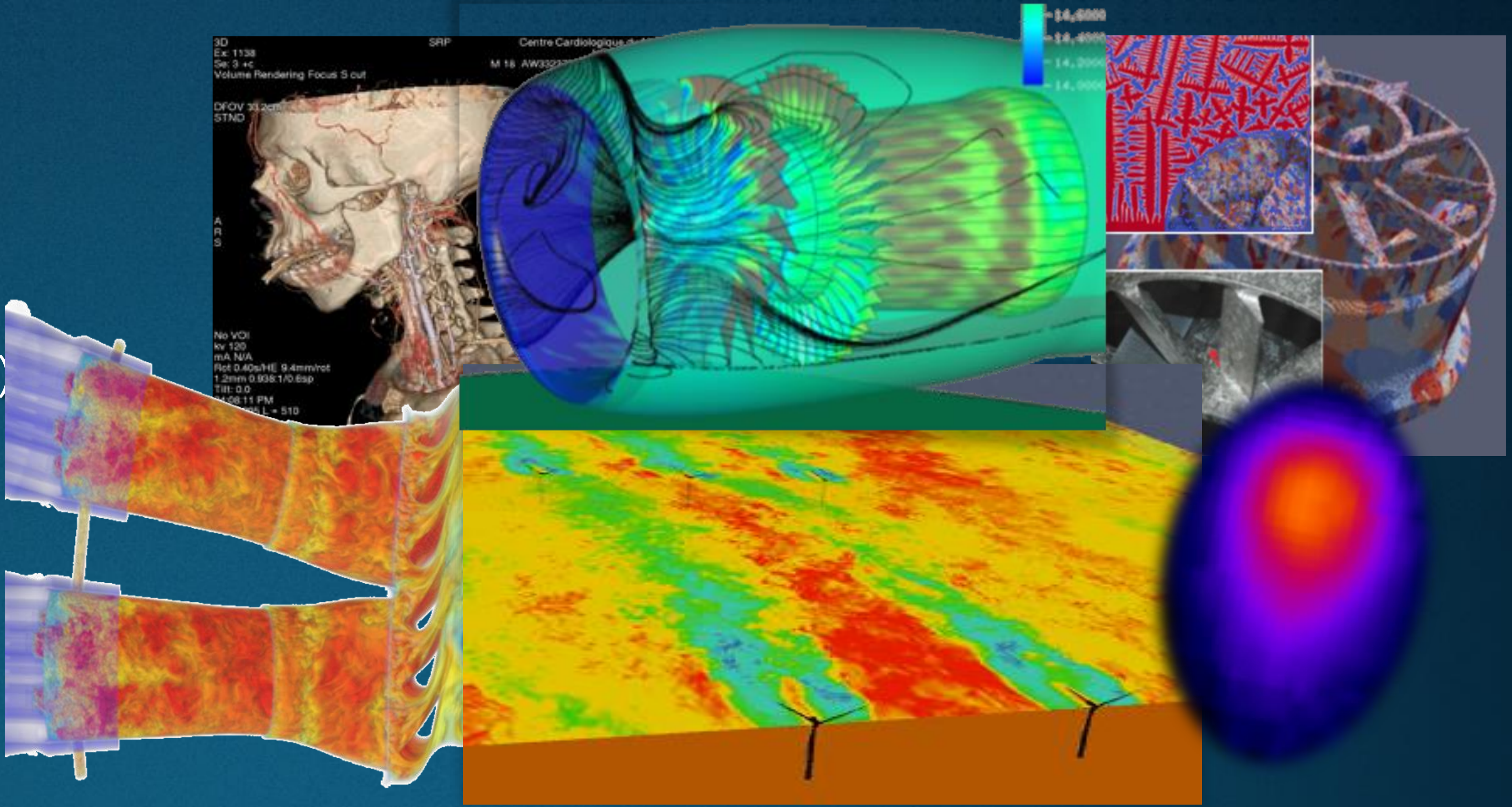
Explore vast alternatives

Modeling & Simulation (Mod/Sim) well-established at GE / GE Research

Computational
Science & Engineering

Gas Turbines | CT scanners | Engines | Wind turbines | Oil & Gas | Additive



Modeling (Form & Function)

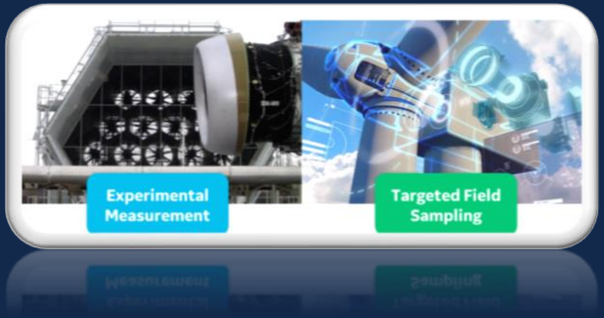
- Geometric Dimensioning & Tolerancing
- Physical Model & Material Properties
- Environment & Operation Conditions

Simulation (Credibility & Confidence)

- Verification & Validation
- Repeatability & Empirical Calibration
- Numerical Assumptions & Effects
- Uncertainty Quantification
- Estimation & Assumption Propagation
- Parametric Sensitivity Analyses

CRITICAL SUPPORT **INFRASTRUCTURE** FOR MODELING

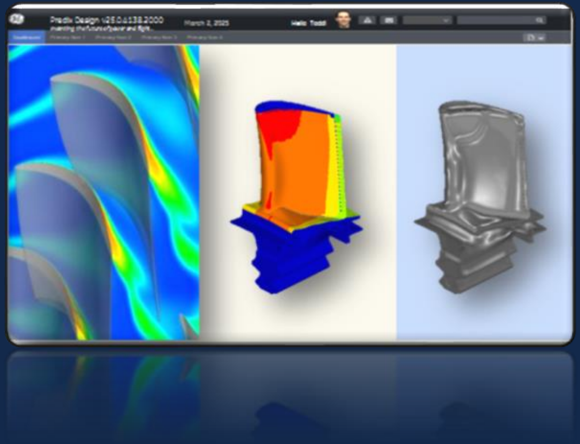
SCIENCE & ENGINEERING INTRUMENTATION



TECHNICAL & REGULATORY PROCESSES

COMPUTATIONAL HARDWARE

SIMULATION & ANALYSIS ECOSYSTEM

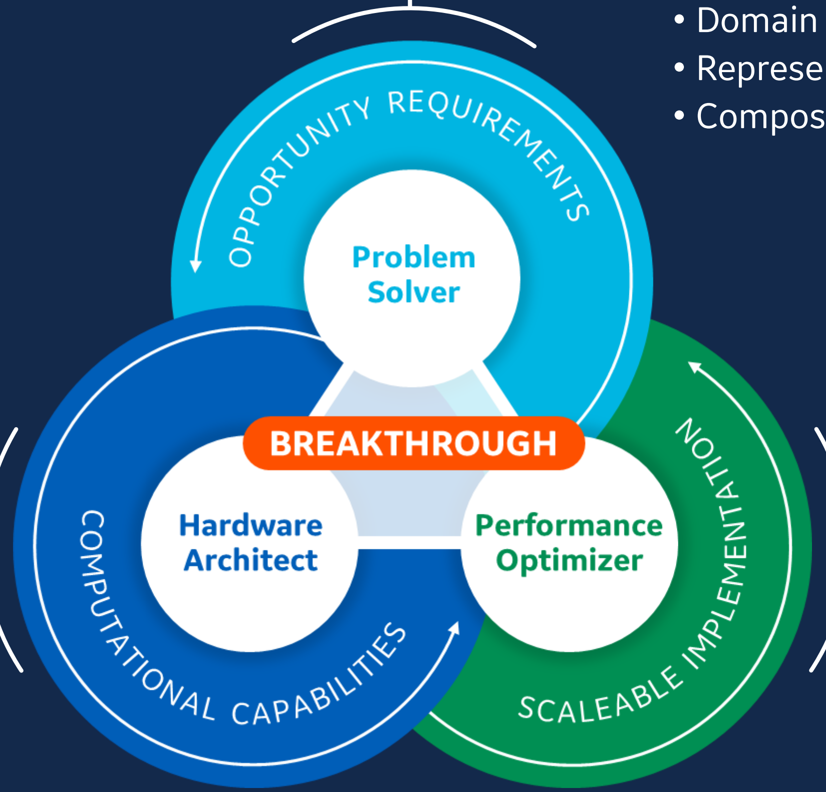


MODEL

- Traceability
- Reproducibility
- Verification & Validation
- Confidence Bounds
- Assumptions, Unknowns & Sources of Error

Co-Design: *A Fugue of Expertise toward Breakthrough Impact*

SCIENCE & ENGINEERING
- Domain Expertise
- Representation Fidelity
- Composition & Comprehension



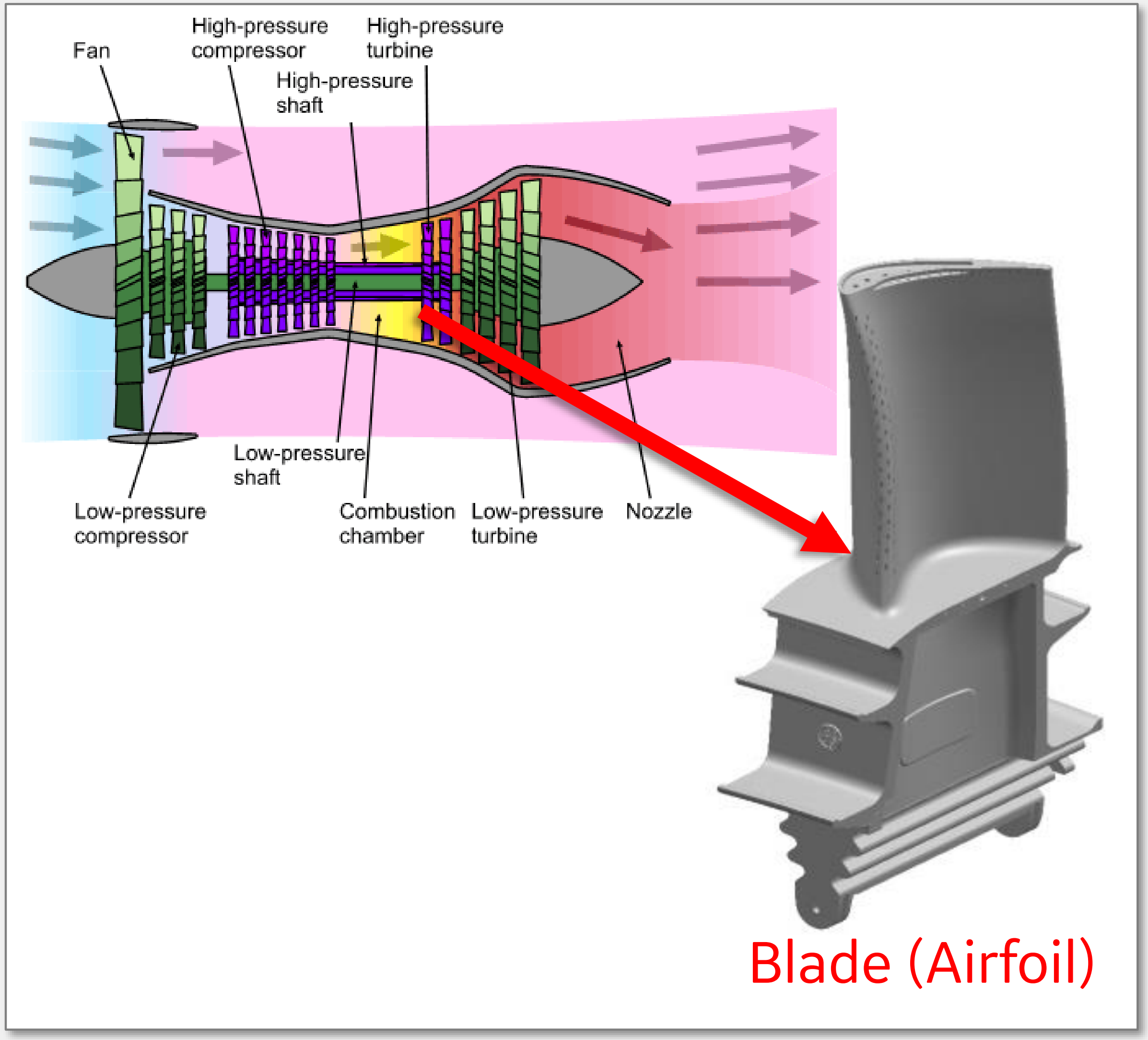
SYSTEMS ENGINEERING
- Vendor Partnerships
- Procurement & Lifecycle
- Infrastructure Tuning

COMPUTATIONAL SCIENCE
- Numerical Methods & Confidence Bounds
- Algorithms & Data Structures
- Productivity & Usability

Product Lifecycle

Conceive → Design → Make → Deliver → Use → Maintain

Brief overview on a core engineering practice at GE:
Design of Blades in Turbomachinery



<u>Objectives</u>:

1. Competitive performance of product *(efficiency, power, …)*
2. Reliability of product *(durability, safety, robust operation)*
3. Cost to design product *(engineering, testing, certification)*
4. Cost to make product *(materials, manufacture, assembly)*
5. Operational cost of product *(including maintenance & repair)*

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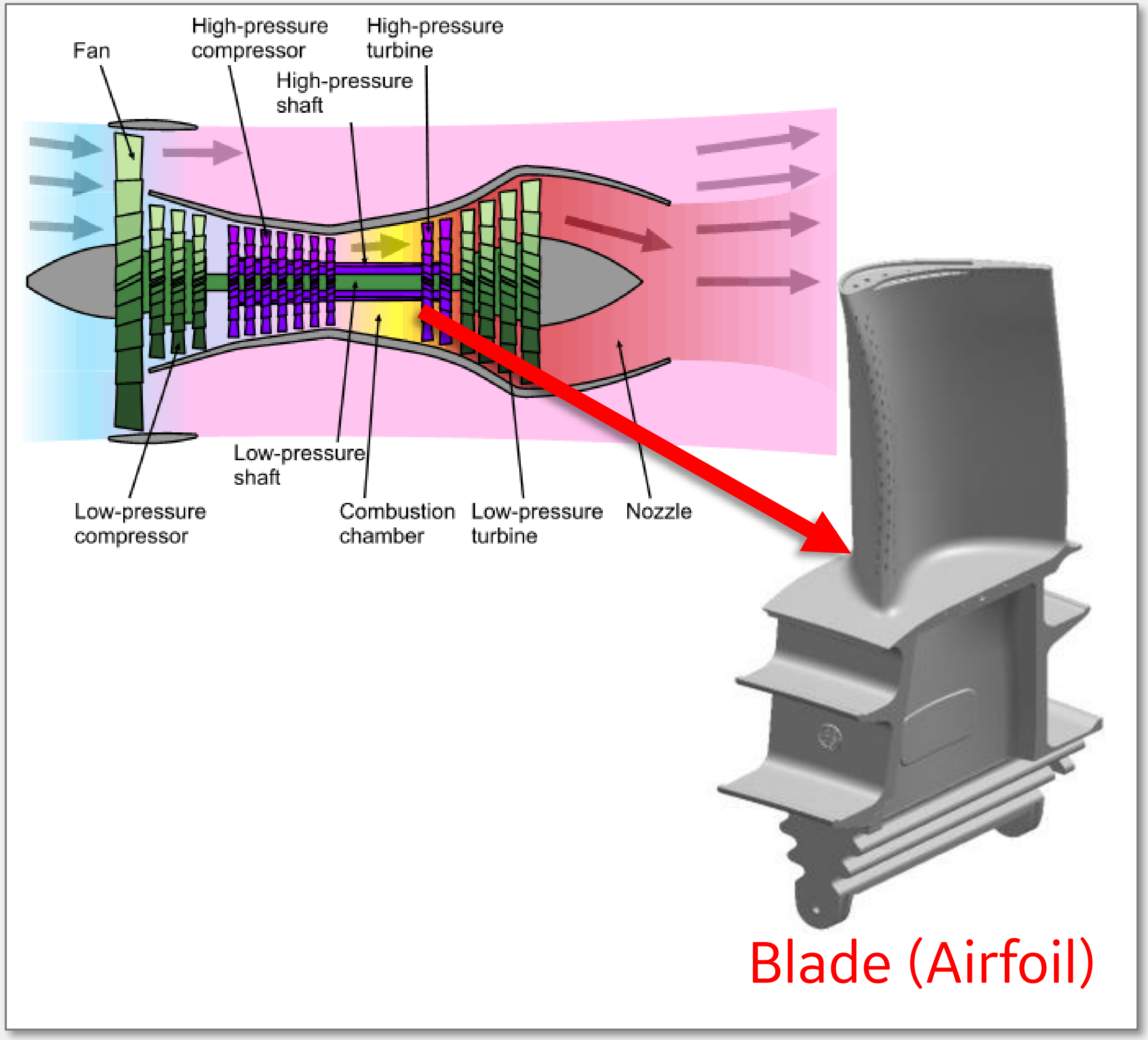
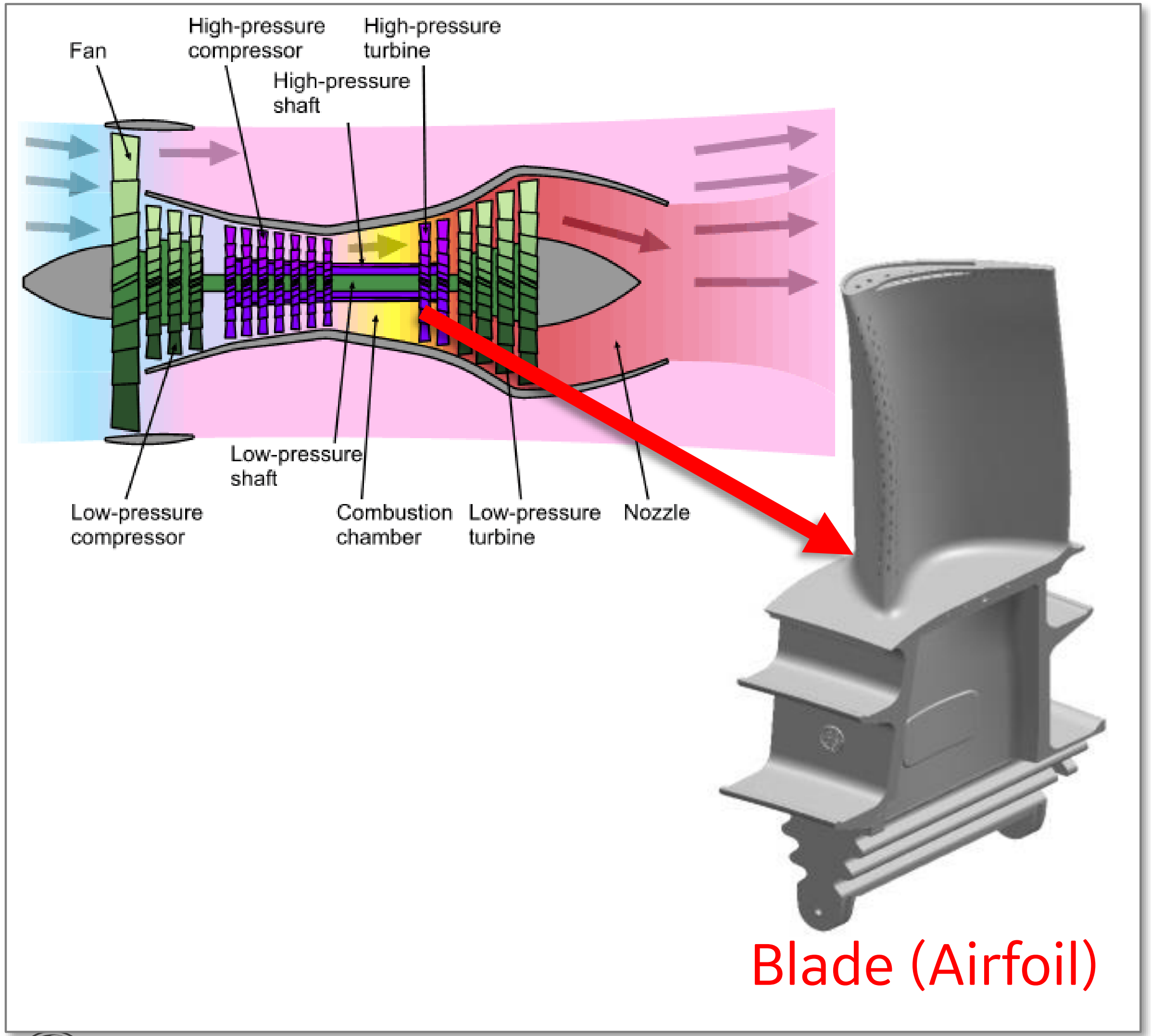


<u>**Objectives**</u>:		<u>**Ideally**</u>:
1. Performance	⬆	Drives Sales (Value for $)
2. Reliability	⬆	Certification on 1st Test
3. Design Cost	⬇	No rework, built to spec+
4. Manufacturing Cost	⬇	No waste, rework, inventory
5. Operating/Service Cost	⬇	Value for $ for customer + GE

Turbine Airfoil Design (*circa 1980*)



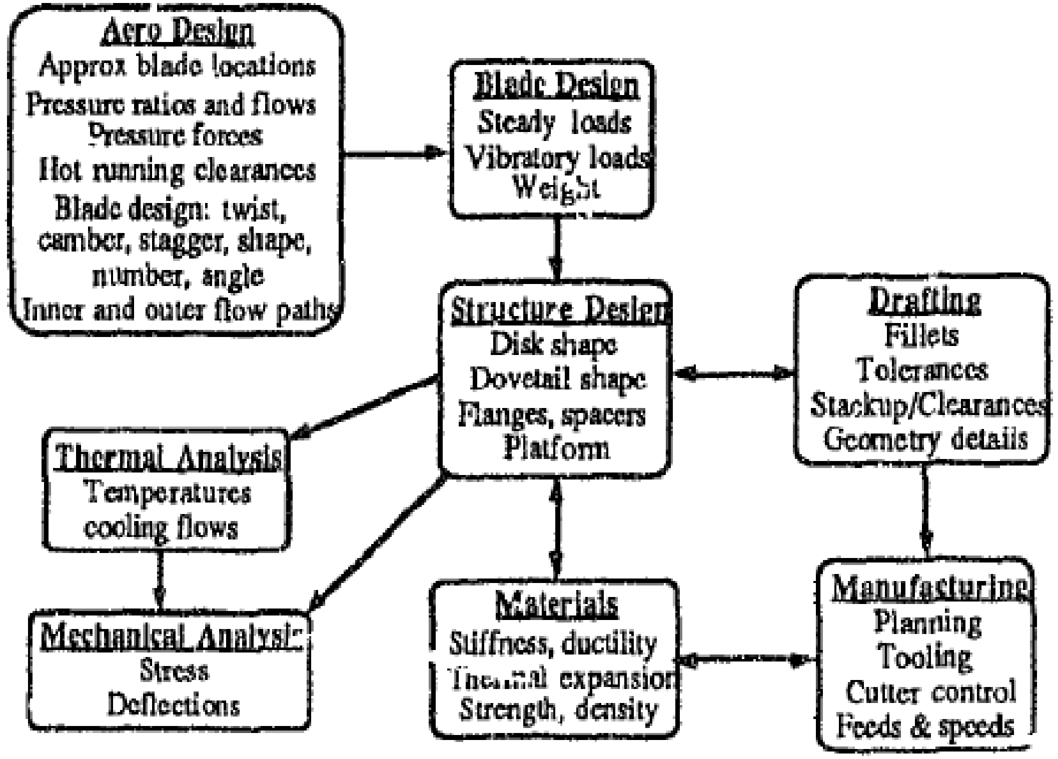
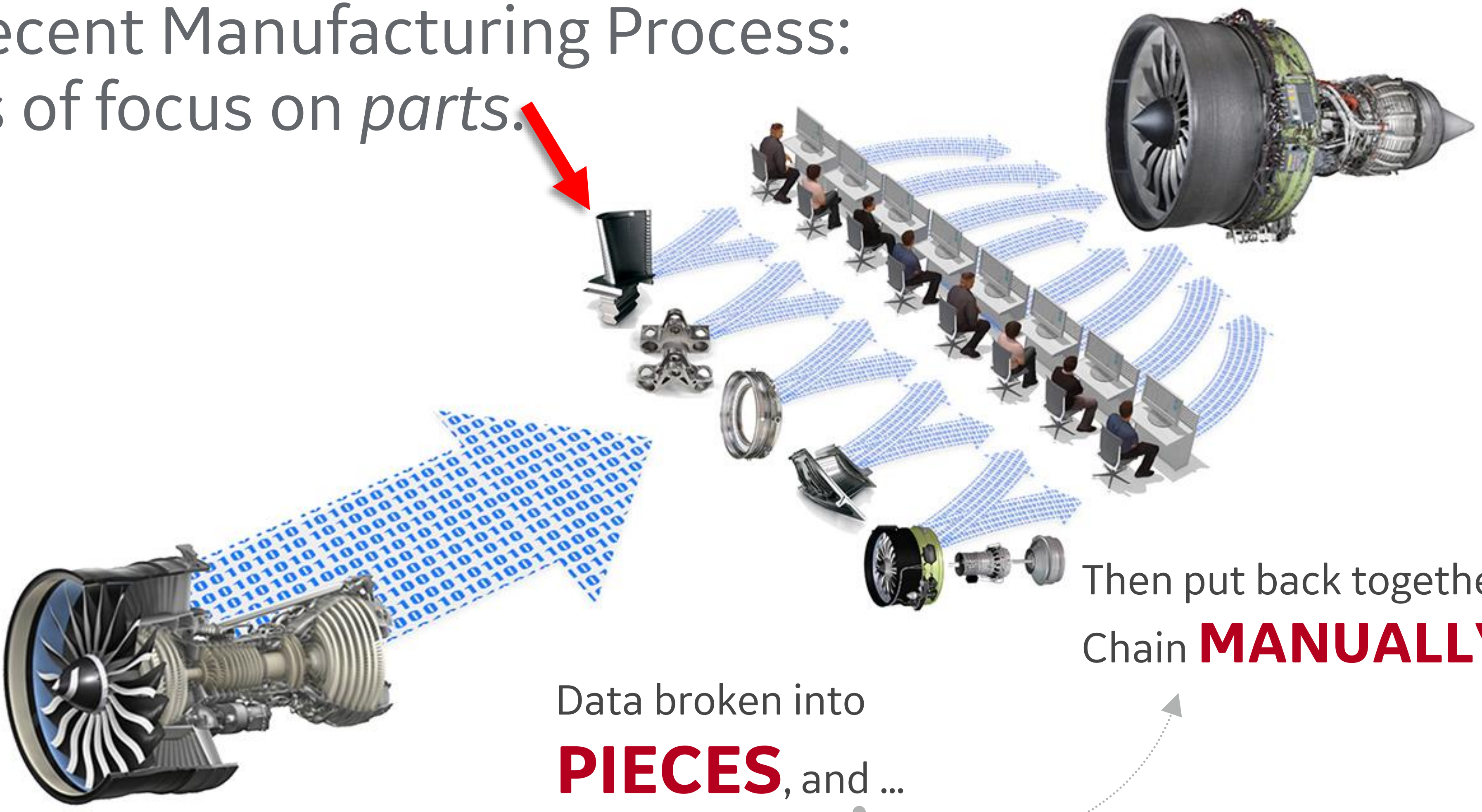


Figure 2. Informal turbine blade design data flow.

More Recent Manufacturing Process: Still lots of focus on *parts*.



Engine designed **DIGITALLY**, but ...

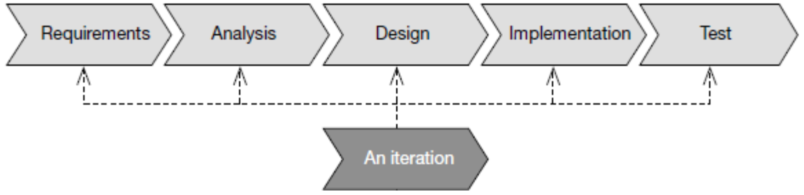
Data broken into **PIECES**, and ...

Then put back together in Supply Chain **MANUALLY**

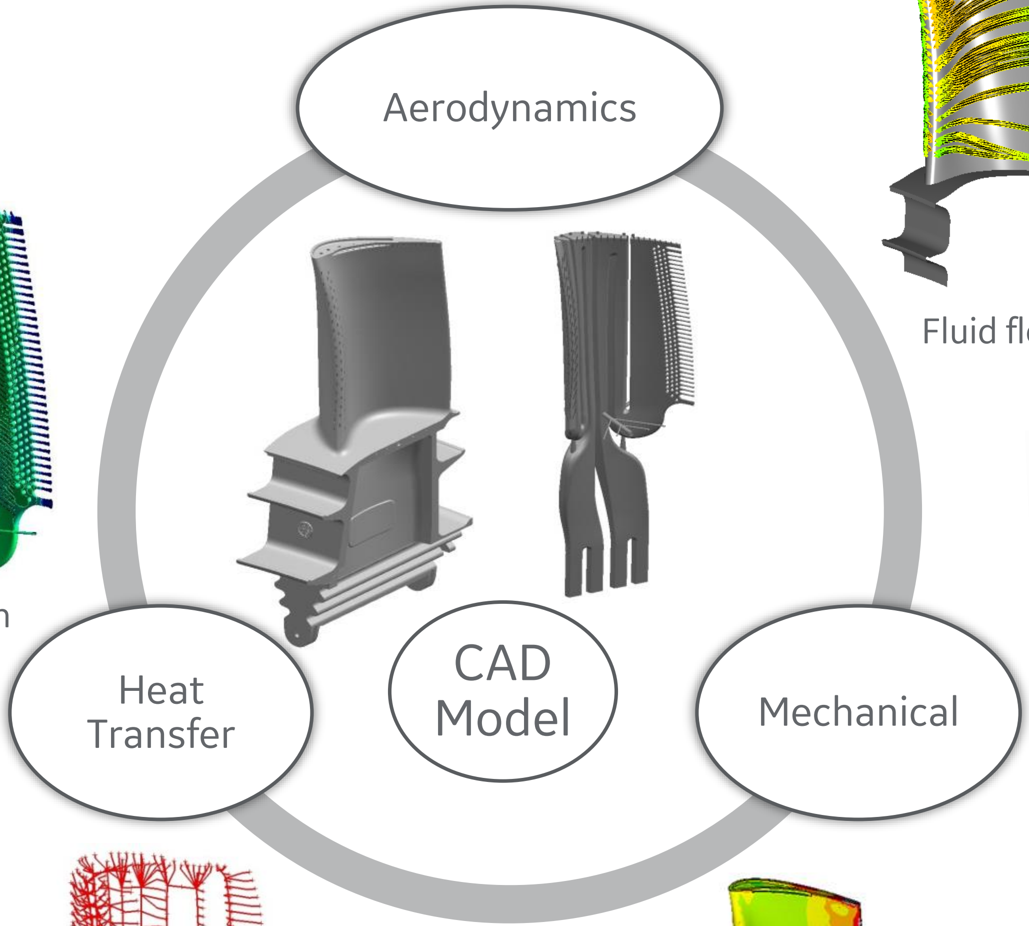
And for part design:
discipline-by-discipline analyses

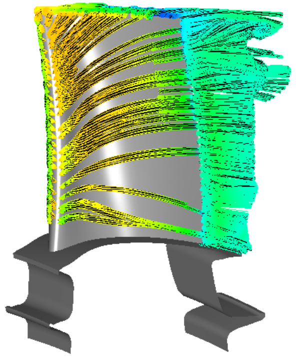
Design Engineering

Each technical stakeholder goes through:

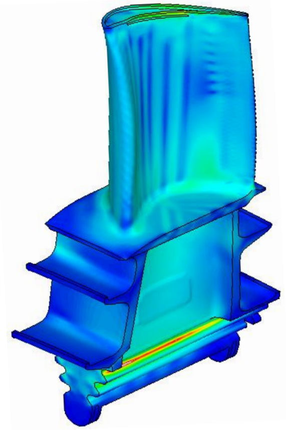


Internal + external design



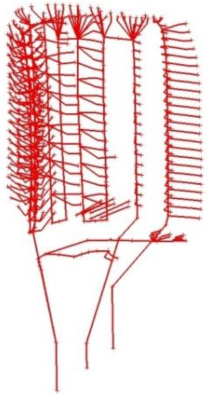


Fluid flow & acoustics

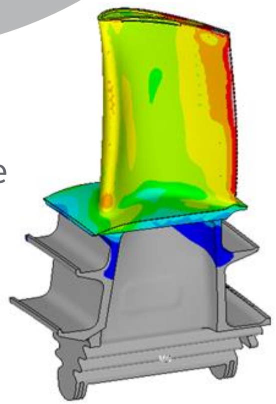


Stress

Internal flow model

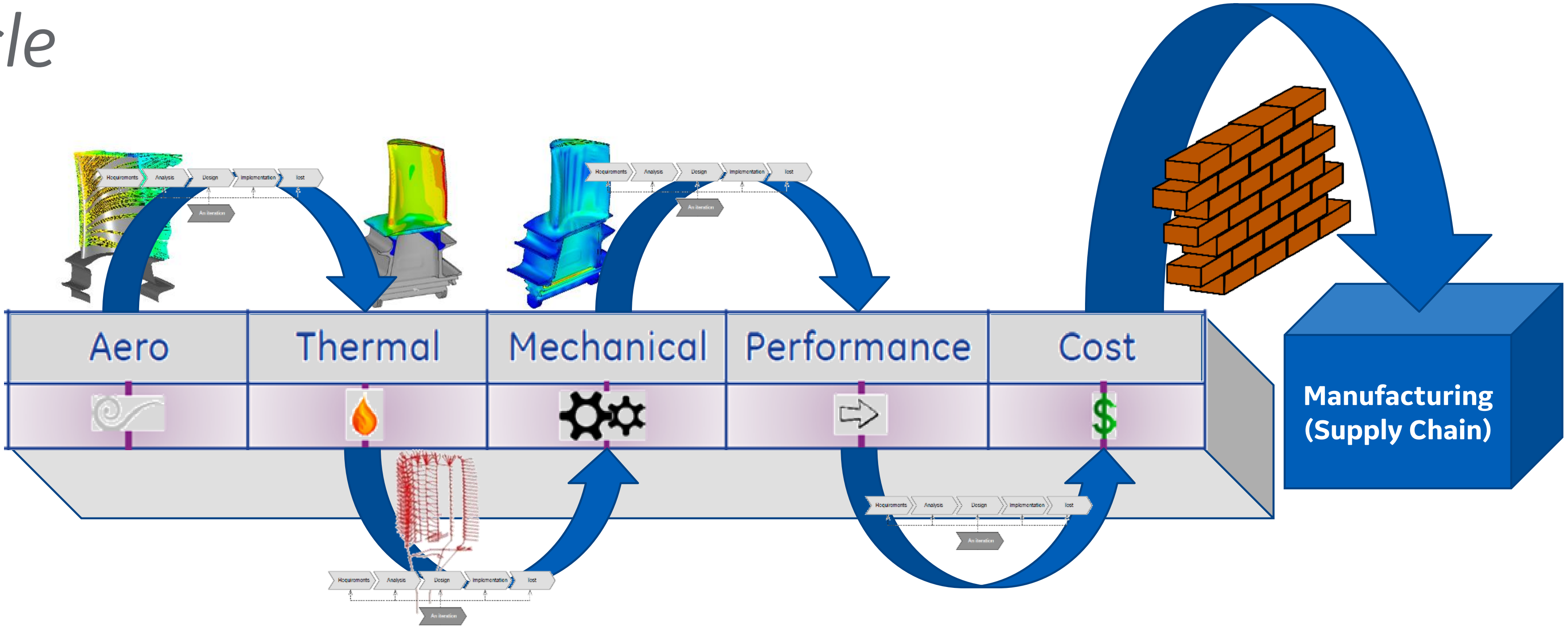


Metal
Temperature



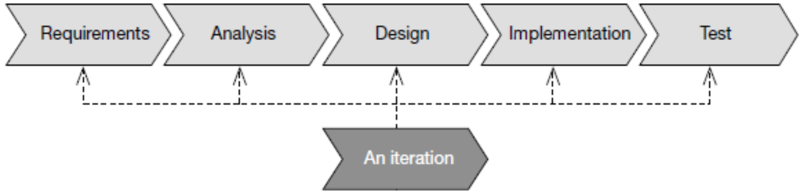
Iterative Design Cycle

Design Engineering



Design hand-offs across disciplines of expertise

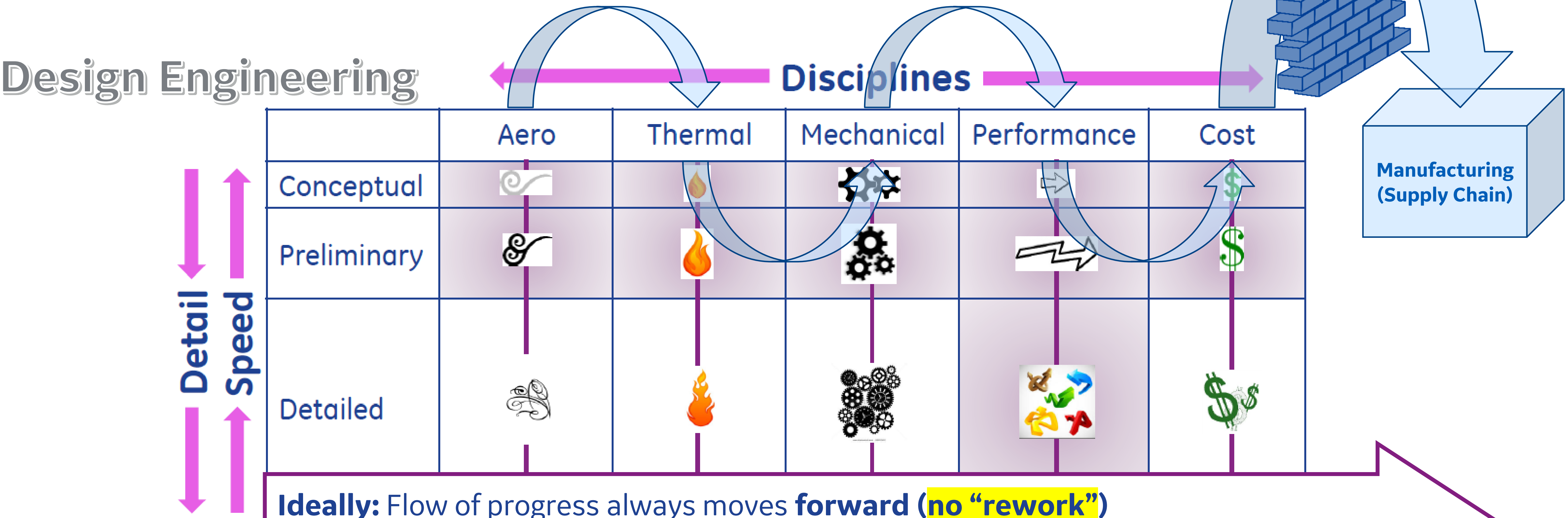
Each technical stakeholder goes through:



"Final Design" handoff to Manufacturing

Example of *Iterative Design Cycle:*

Each engineering domain expert designs to requirements for their discipline.

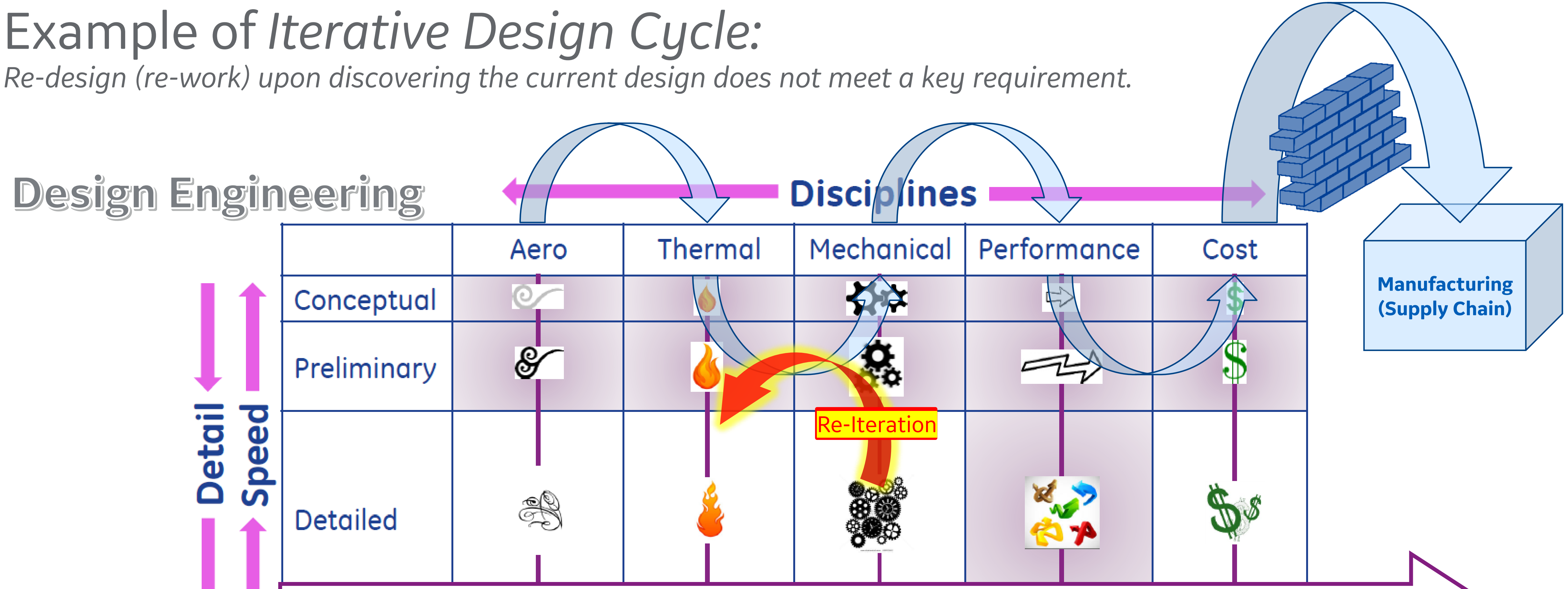


Ideally: Flow of progress always moves **forward (no “rework”)**

- Fully Integrated data representation
- Common tools for all levels of detail (trade off precision and speed without impacting accuracy)
- Design flaws (such as contradictions across stakeholder disciplines) minimally reverse progress

Example of *Iterative Design Cycle:*

Re-design (re-work) upon discovering the current design does not meet a key requirement.



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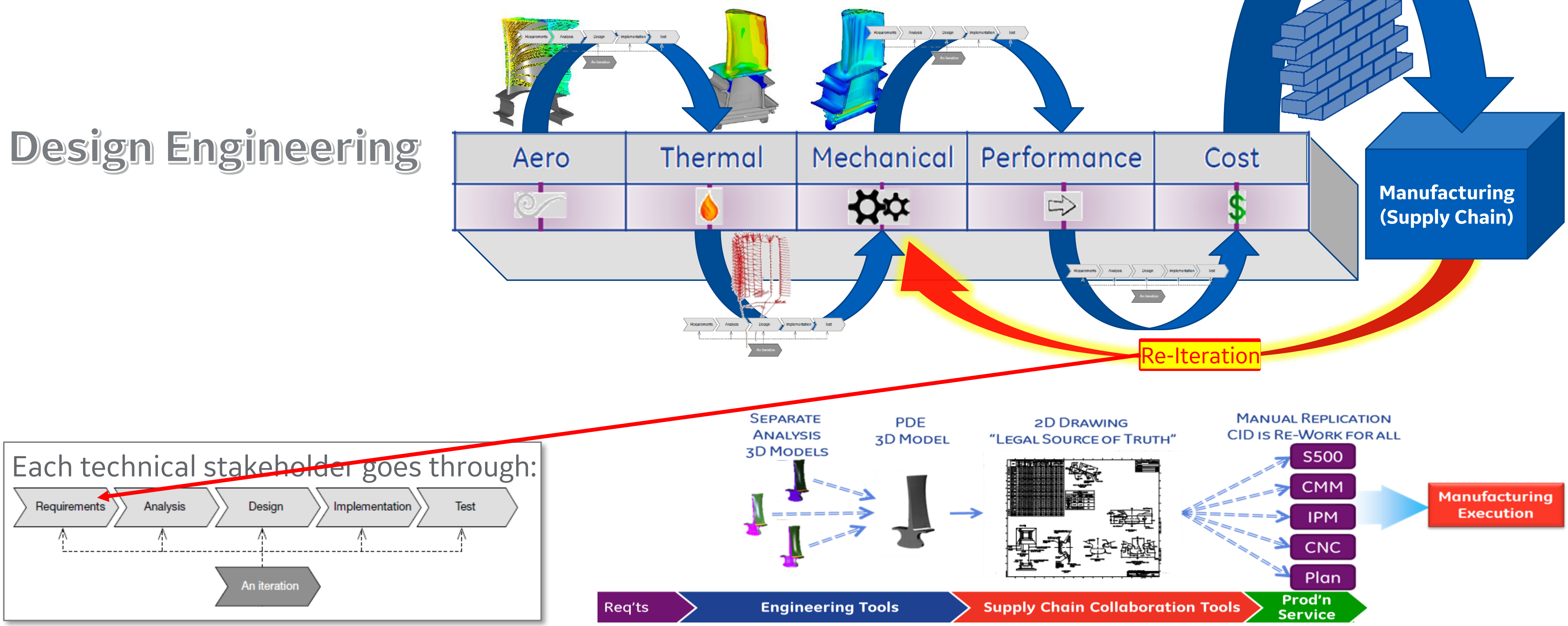
Iterative Design-to-Manufacturing Cycle

Parts not feasibly/reliably/cost-effectively manufactured may also kick back to re-work.



Digital Thread & "The Shadow of Design"

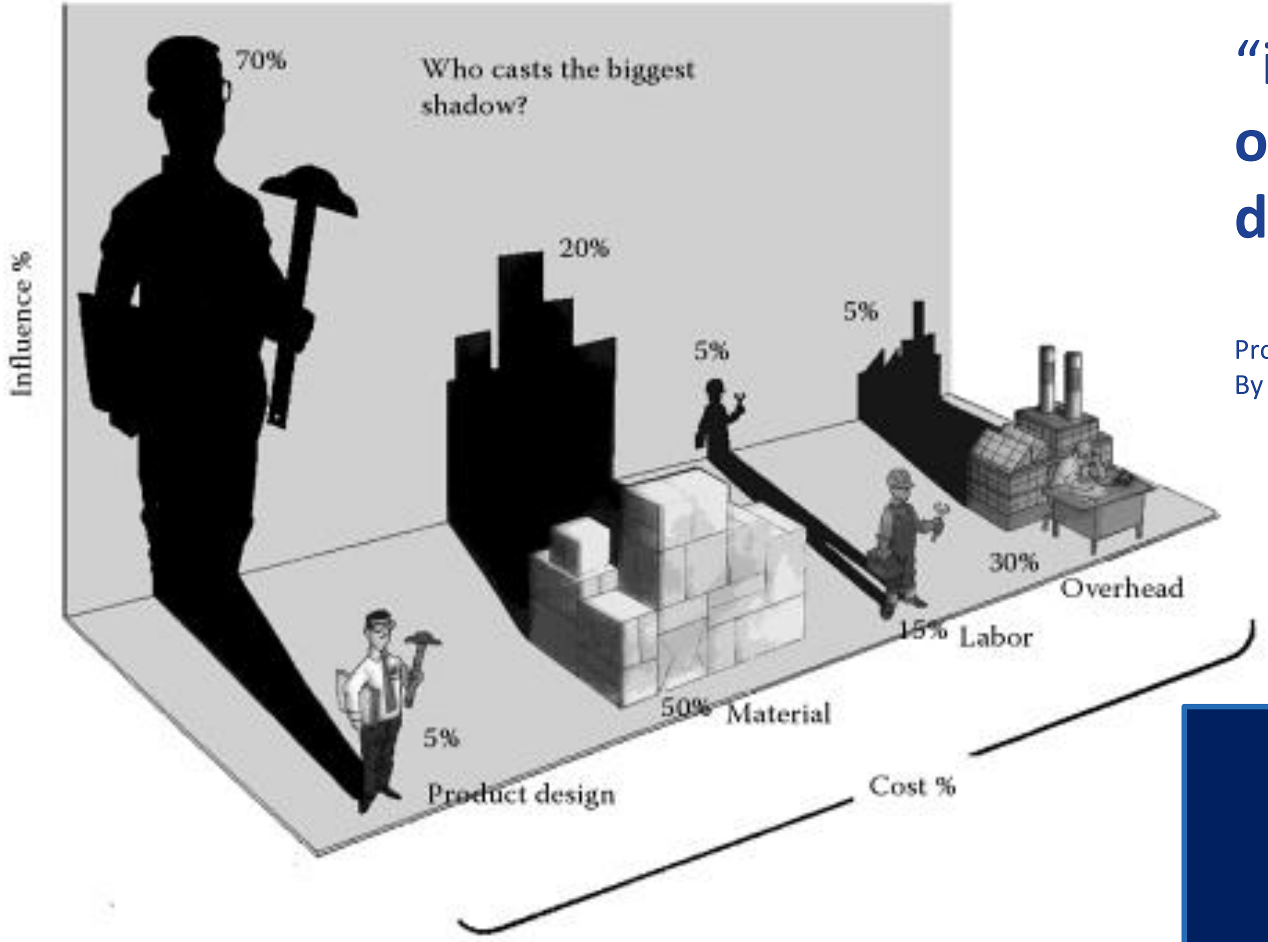


FIGURE 1.5
Who casts the biggest shadow? (Adapted from Munro and Associates, Inc.)

"it is now widely accepted that **over 70% of the final product costs are determined during design**"

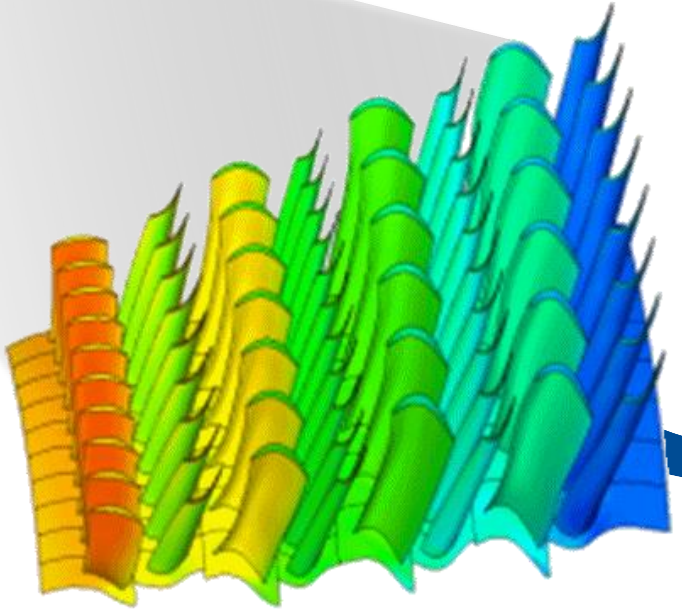
Product Design for Manufacture and Assembly, Third Edition
By G. Boothroyd, P. Dewhurst, V. A. Knight

Drive **Variable Cost Productivity (VCP)**
by
pushing **cost visibility** into Design

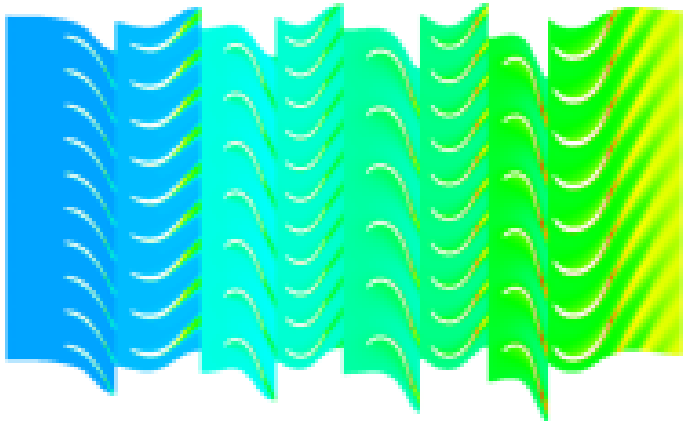
GE Impact leveraging Leadership Computing

High-end modeling - Moment of truth

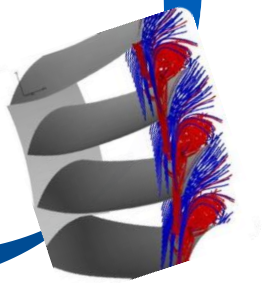
Will we see
something different?



Will it be
useful?



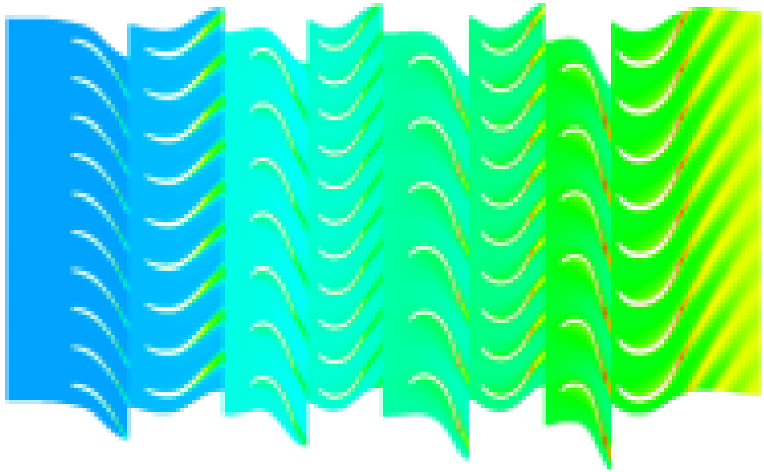
Compare:
Best Internal
Modeling
Capability



GE Aviation LEAP
Unsteady CFD: Strut wake effects
GE Tacoma RANS solver

Never before seen

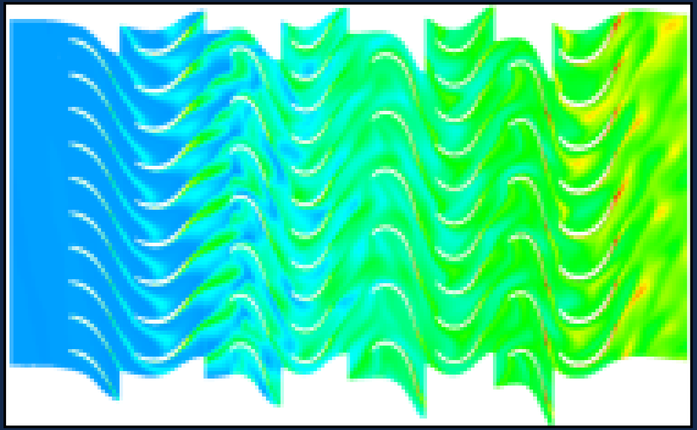
- Unobservable physically
- Relevant to engineering design
- 2012 IDC award:

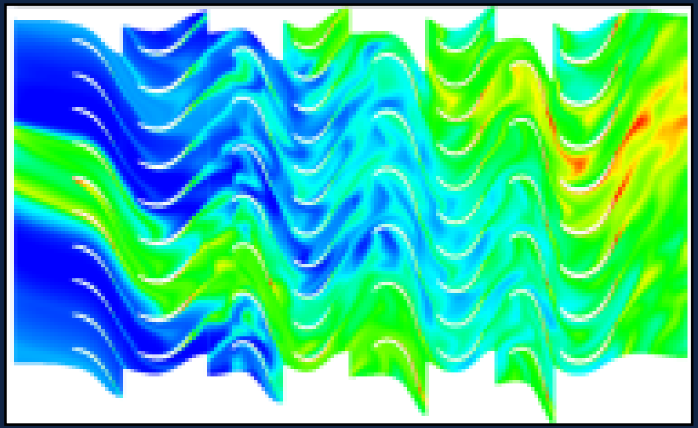


Prior State of the Art:
Steady Analysis
(GE Internal HPC)

On ORNL Jaguar Cray XT5 (2010)

Preliminary Result
Unsteady Analysis
(with Uniform Inlet)





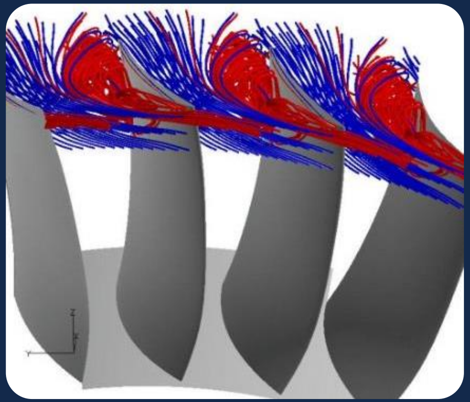
Final Result
Unsteady Analysis
(with wake from strut)

Software: Simulation and Modeling

Dynamic Flows

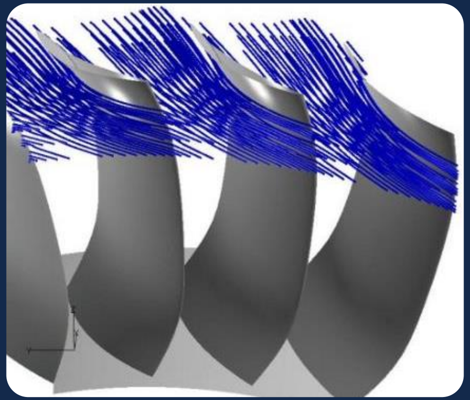
- Heat
- Acoustics
- Fuel Burn
- Emissions

Separated flow - poor air flow control and loss of efficiency



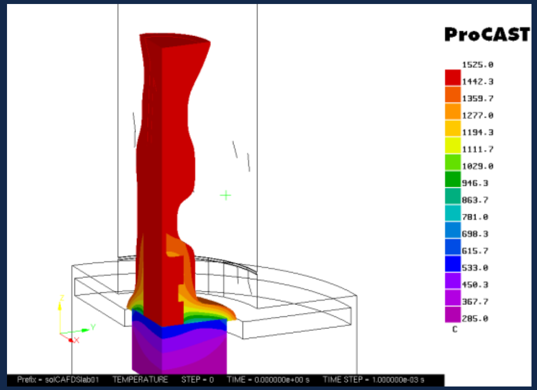
Old Design "Straight Airfoil"

Attached flow - good air flow control and high efficiency



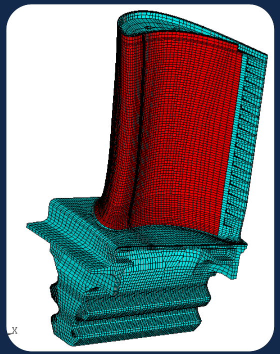
New Design Using "Bowed Airfoil"

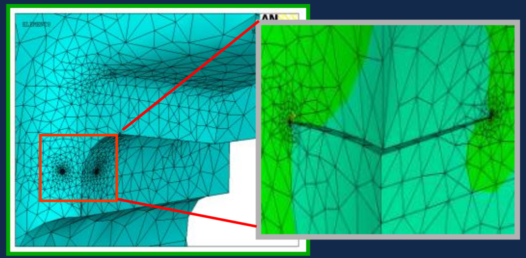
Material Design



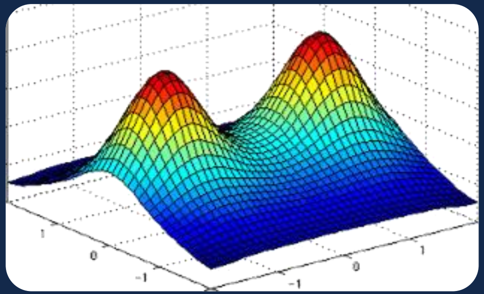
Mechanical Properties

- Metal alloy wear and tear
- "Crash tests" (bird strike)





Design Optimization



Computational Methods Maturity

a.k.a. Virtual / Digital / Computational / Numerical Modeling

Criticality *of Computational Modeling*

- *All* problem-solving employs *models*
  (even if merely mental models of the person solving).
- Some problems necessarily must be modeled *computationally* due to factors such as physical test expense/difficulty/safety, turnaround time, legality/ethics, and/or measurement limitations.

Critique *of Modeling*

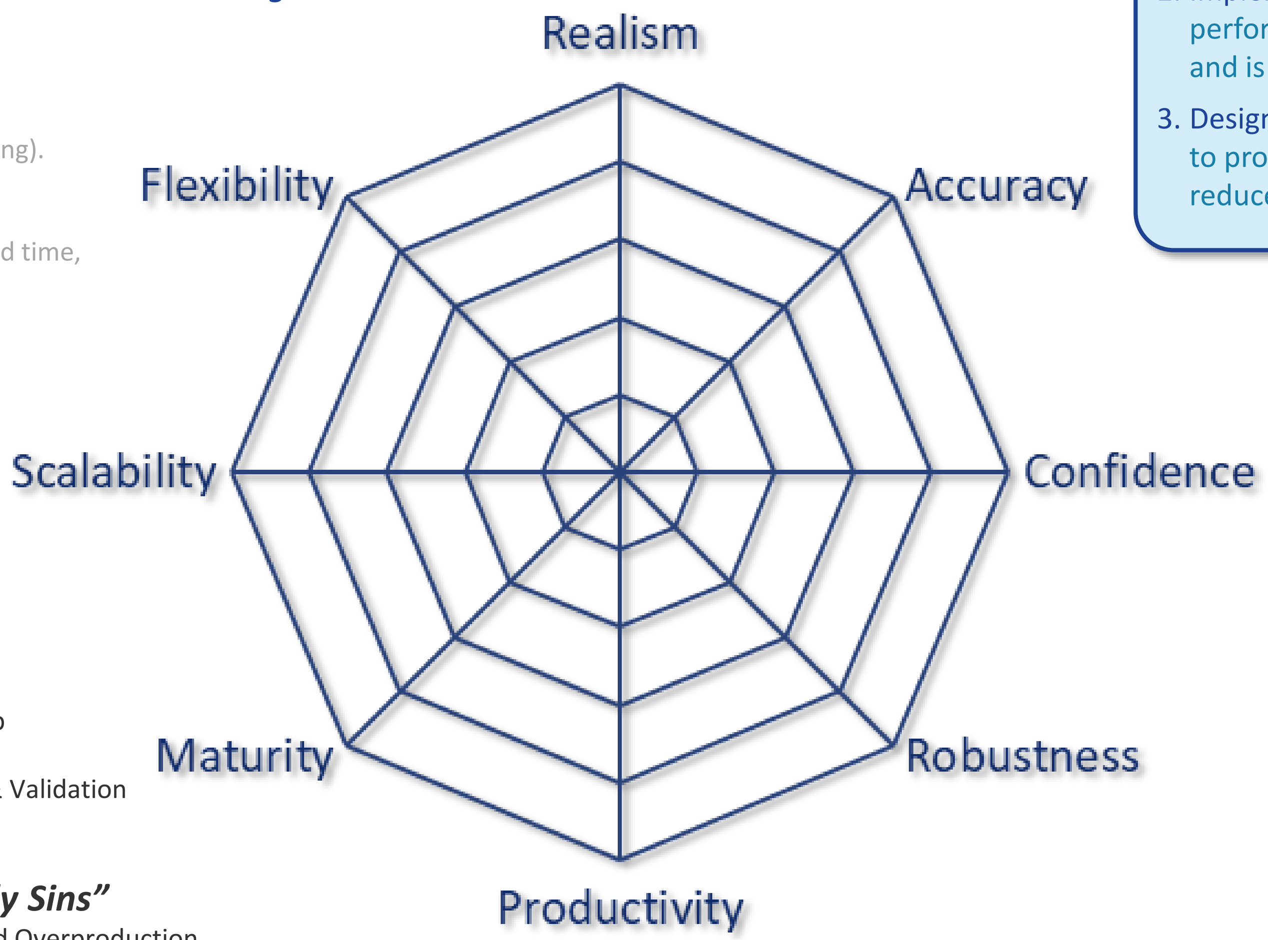
- Garbage-in = Garbage-out
- To advise and inform *decision-making,* models must be *trusted* and *understood* by both the people composing the models as well as those interpreting the models.

Crucial *to Computational Modeling*

- Computationally Literate Workforce & Leadership
- Hardware & Software Infrastructure & Ecosystem
- Facilities, Processes and Culture for Verification & Validation

Digital Opportunities vs. ***LEAN's "Deadly Sins"***

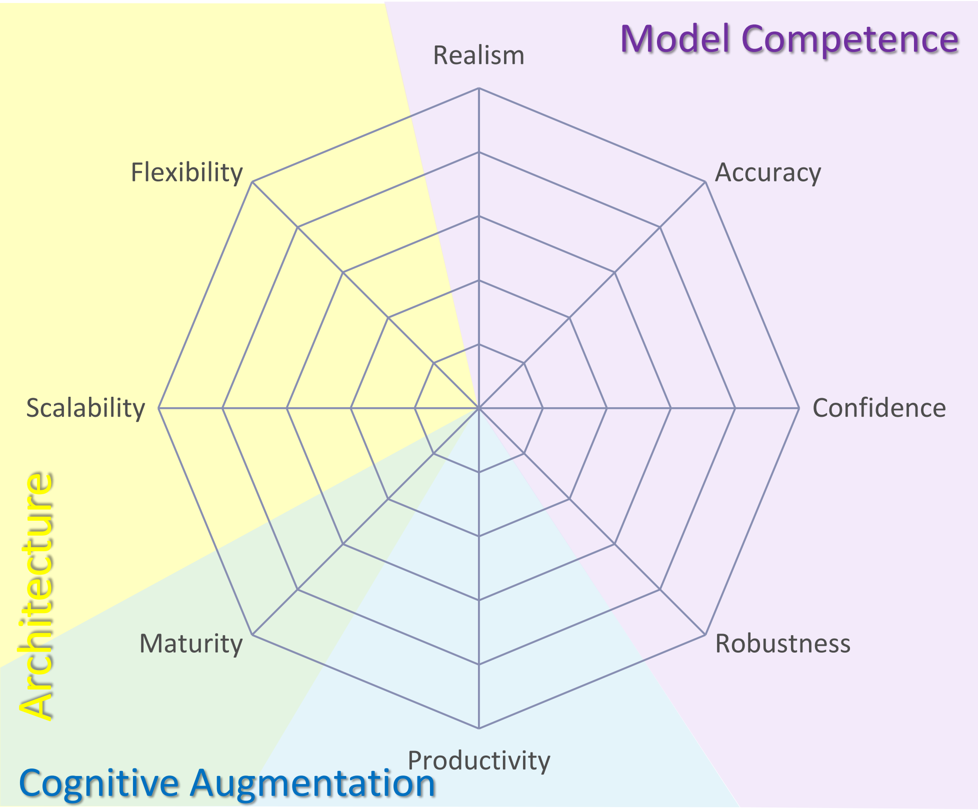
- Reusable Virtualized Assets vs. Inventory/WIP and Overproduction
- Automation & Visibility to increase Productivity and reduce Waste / Defects / Rework
- Digital Thread Workflow vs. Motion/Waiting dependencies/hand-offs and Underused Talent



Computational Modeling Goals

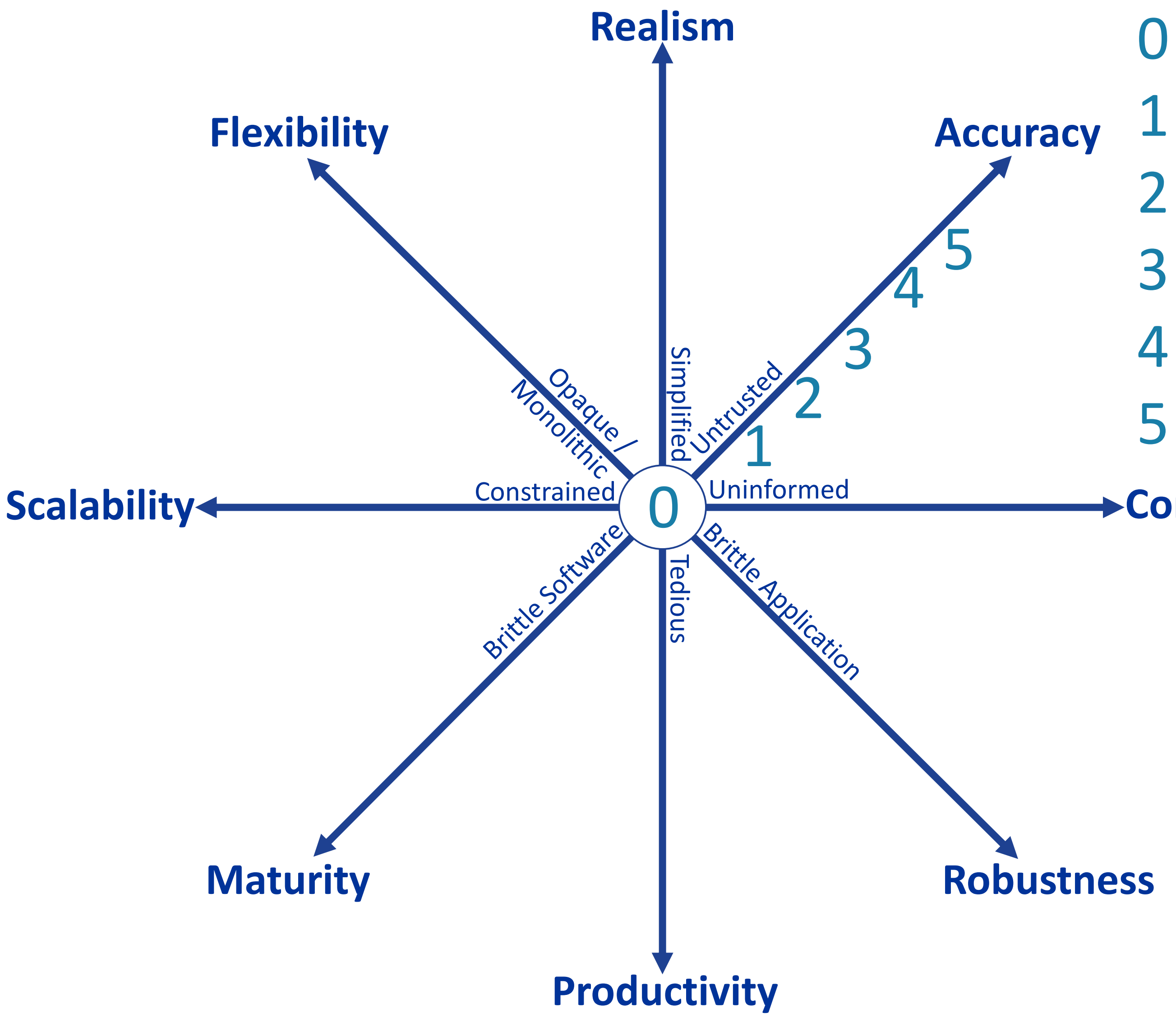
1. Assert a ***Region of Competence*** for a model where its use is numerically stable (**ROBUSTNESS**) with minimal simplifying constraints (**REALISM**) and quantifiably bounds uncertainties (**CONFIDENCE**) of results with validated predictive **ACCURACY**.
2. Implement the model with an ***Architecture*** that performs capably on HPC hardware (**SCALABILITY**) and is interoperable and extensible (**FLEXIBILITY**).
3. Design model use and software management to promote efficient workflows (**PRODUCTIVITY**), reduce waste and improve quality (**MATURITY**).

Co-Design Web: Goals

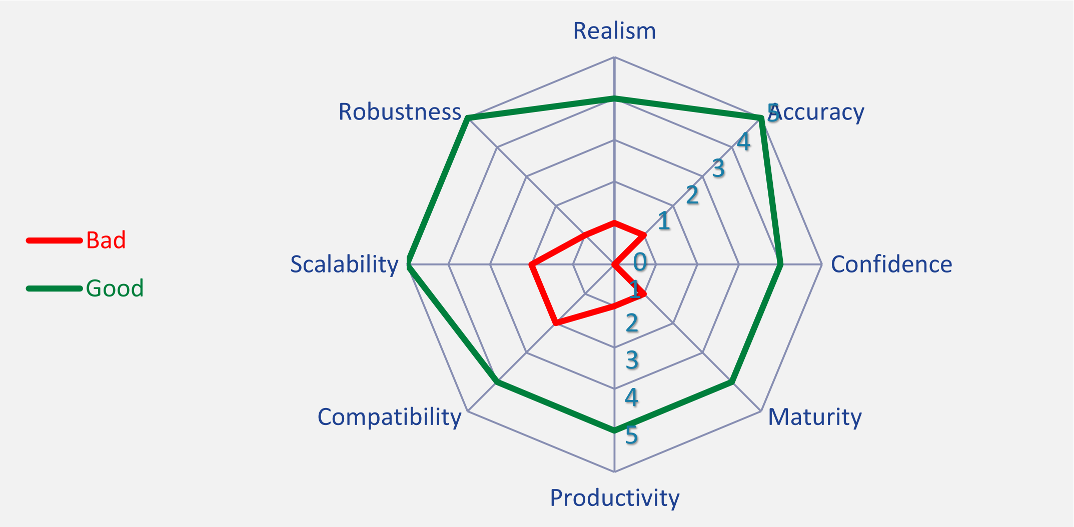


Realism	*Completeness of …*	*… Model's Region of Competence*
Accuracy	*Validity within…*	
Confidence	*Error bounding within…*	
Robustness	*Stability & Assertability of…*	
Productivity	Cognitive Augmentation	*& Waste Reduction*
Maturity		*& Architecture Quality*
Scalability	*Capable & High Performance*	Architecture
Flexibility	*Modular, Extensible, Interoperable*	

Co-Design Web: Measurement



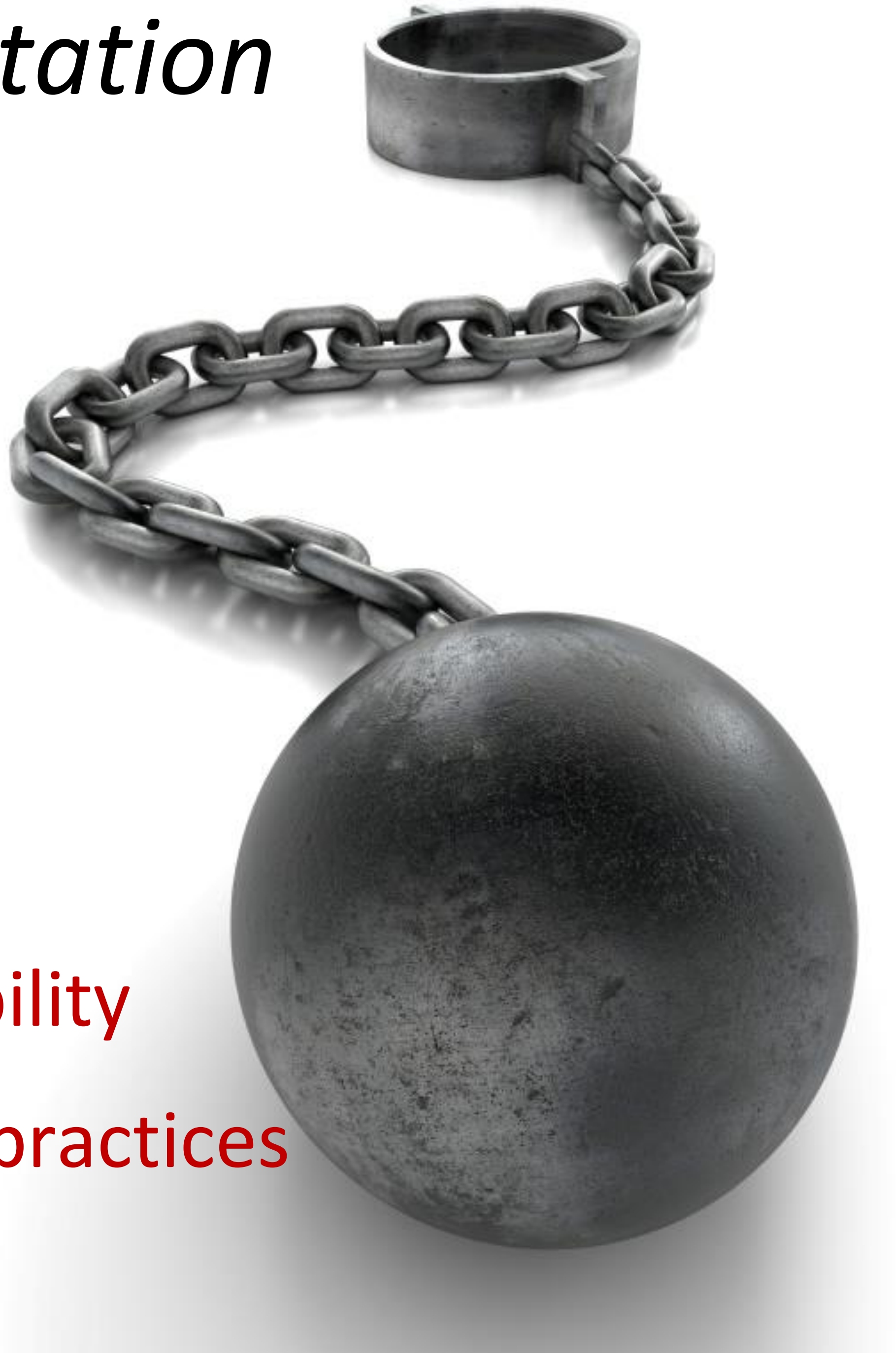
0 = **Undesirable** (Absent)
1 = Minimally present
2 = Documented / Basic
3 = Managed & Consistent / Addressed
4 = Systemic & Repeatable / Advanced
5 = **Best in Class** / State of the Art



Challenges

Challenge: Legacy

Legacy: *Strength* becomes *Limitation*



- ✓ Experience
- ✓ Confidence
- ✓ Regulatory acceptance
- ❖ Sunk investments deter re-investment
- ➢ Obsolete functionality / infrastructure
- ➢ Cost/complexity for backward compatibility
- ➢ Hinders innovation / adoption of novel practices


Data Lake

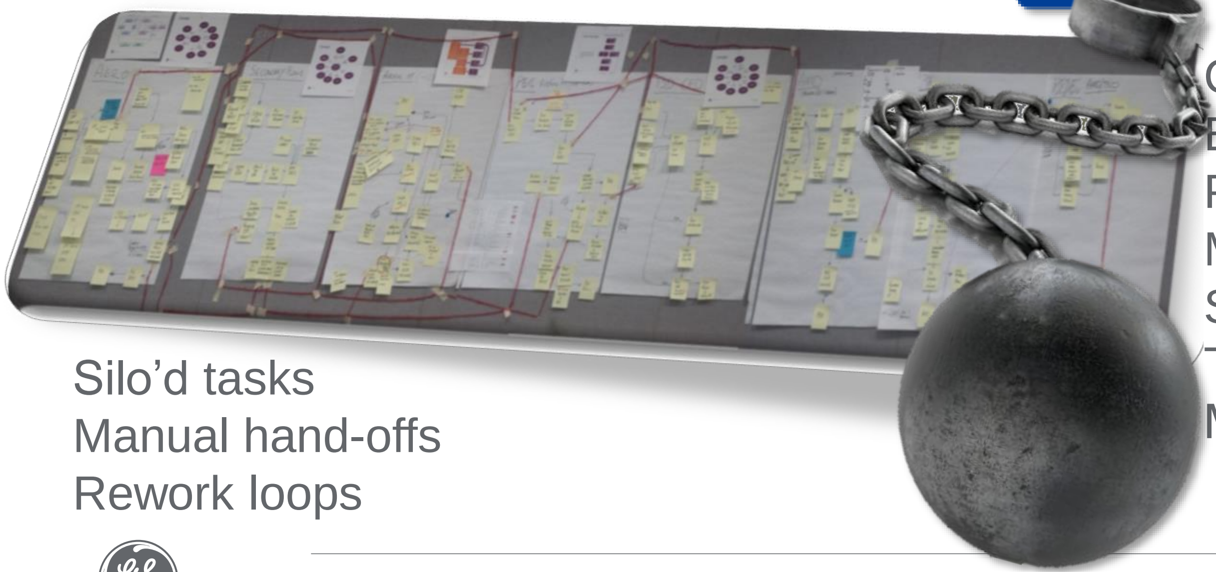
Data Lake Storage & Services Infrastructure

DIGITAL THREAD CENTRALIZATION/FEDERATION OF LEGACY DATA / SOFTWARE

- CRM data … SIEBEL, salesforce …
- ERP data … SAP, ORACLE …
- PLM data … ENOVIA, TEAMCENTER …
- MES data … GE, SIEMENS …
- Simulation data … ANSYS, MathWorks … + ML data theano …
- Test data … NATIONAL INSTRUMENTS, KEYSIGHT TECHNOLOGIES …
- MRO data… GE, IBM …

Data Lake Storage & Services Infrastructure

DIGITAL THREAD SOURCES FROM **LEGACY WORKFLOWS / PROCESSES**

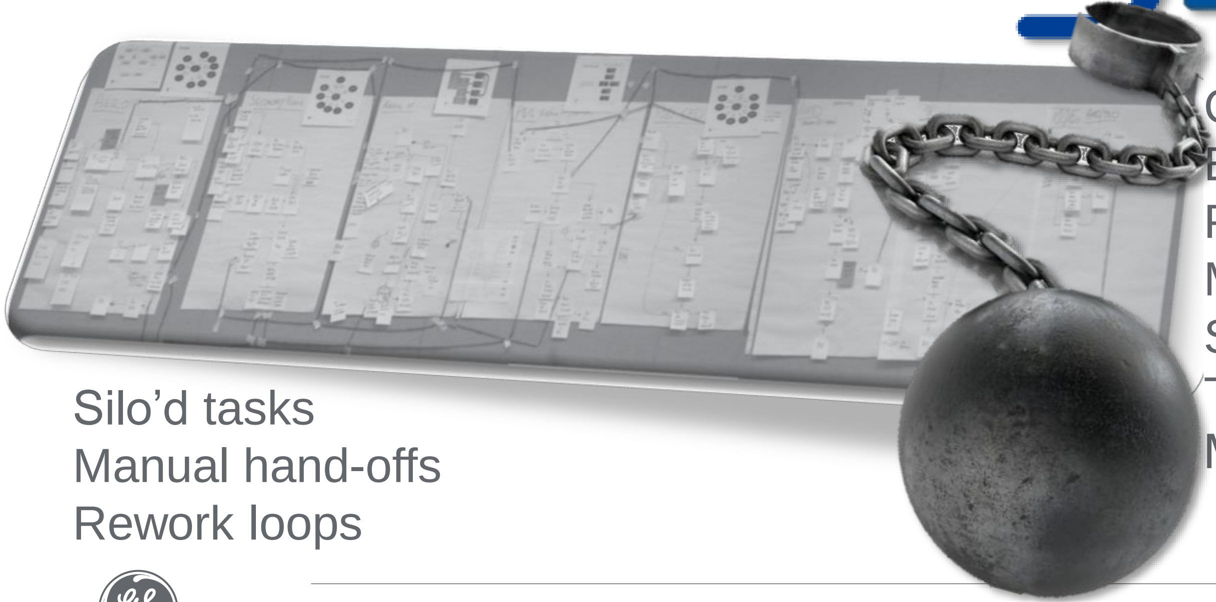


CRM data	SIEBEL	salesforce	…
ERP data	SAP	ORACLE	…
PLM data	ENOVIA	TEAMCENTER	…
MES data	GE	SIEMENS	…
Simulation data	ANSYS	MathWorks	… + ML data theano …
Test data	NATIONAL INSTRUMENTS	KEYSIGHT TECHNOLOGIES	…
MRO data…	GE	IBM	…

Silo'd tasks
Manual hand-offs
Rework loops

Data Lake Storage & Services Infrastructure

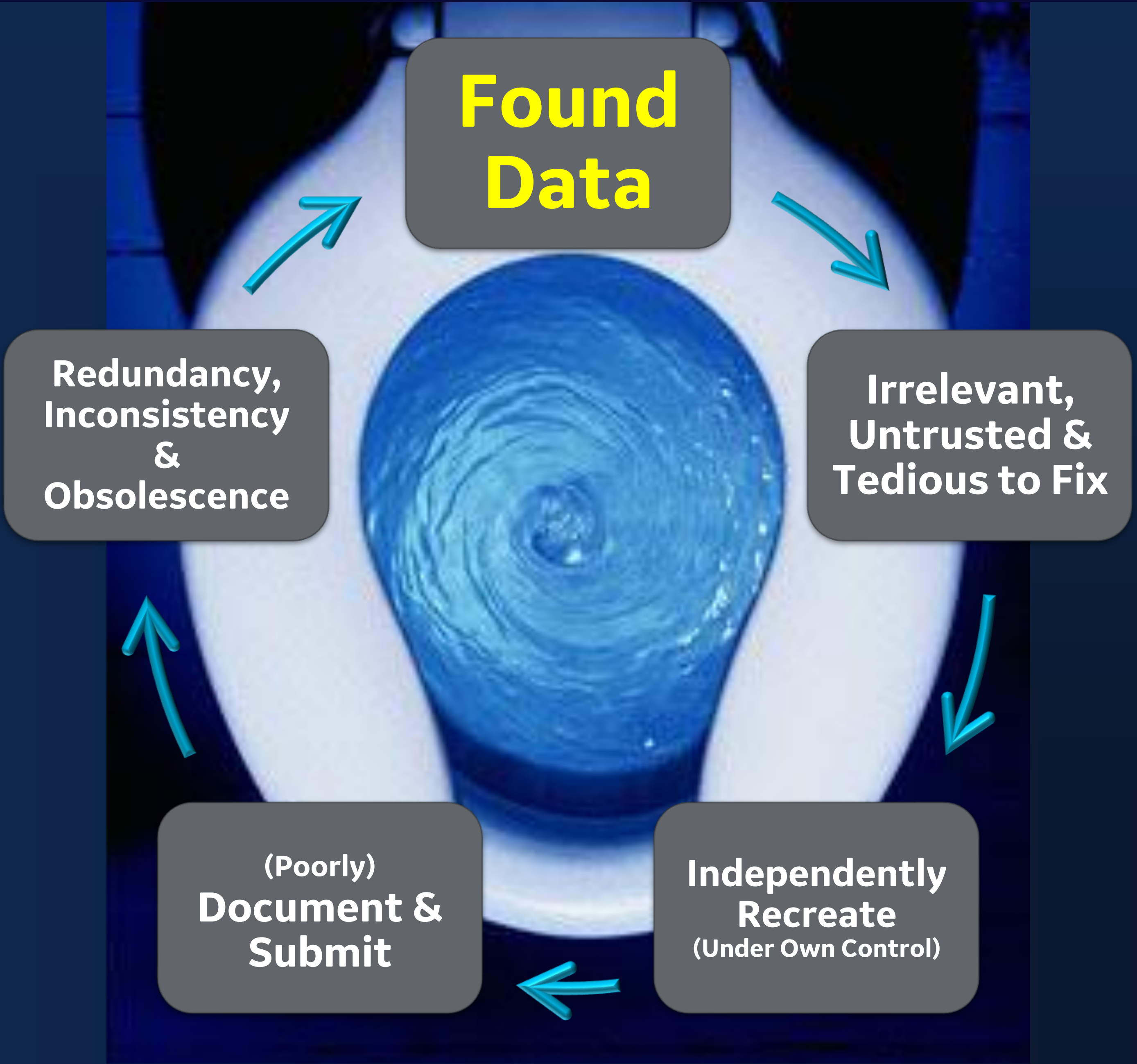
INDEXING, SEARCH, REPORTING, PROTECTION & COMPLIANCE



CRM data …
ERP data …
PLM data …
MES data …
Simulation data … + ML data theano …
Test data …
MRO data… …

Silo'd tasks
Manual hand-offs
Rework loops

CHALLENGE: VICIOUS CYCLE OF DATA DEGRADATION




Data Swamp
Challenge

Opportunity: Decision Provenance *– akin to "Design Rationale" concept*

DECISIONS AS "PRIMARY INDEX" TO UNDERLYING DATA/ANALYSES

At time of DECISION,

explicitly capture into *knowledge steward*:

prov·e·nance
/ˈprävənəns/

noun
noun: **provenance**

the place of origin or earliest known history of something.
"an orange rug of Iranian provenance"
synonyms: origin, source, place of origin; More

- the beginning of something's existence; something's origin.
  "they try to understand the whole universe, its provenance and fate"
- a record of ownership of a work of art or an antique, used as a guide to authenticity or quality.
  plural noun: **provenances**
  "the manuscript has a distinguished provenance"

Who	Proposed, Reviewed, Approved, Tested?
What	Alternatives were considered? Known Unknowns *(environmental, economic, …)*
Why	Assumptions *(limitations, dependencies, technology, …)* Evaluation Criteria & relative weights (and then *link* to underlying references):
How	Data analyses supporting the decision Modeling methods applied (+ intellectual debt) Physical process for measurement *(Gage R&R, …)* Future footnotes: exemplar practices / learnings *and opportunities to improve (given more time/budget/capability)*

Challenge: Machine Learning Reference Data

SUFFICIENCY FOR TRAINING

Complexity of Response Hyper-surfaces

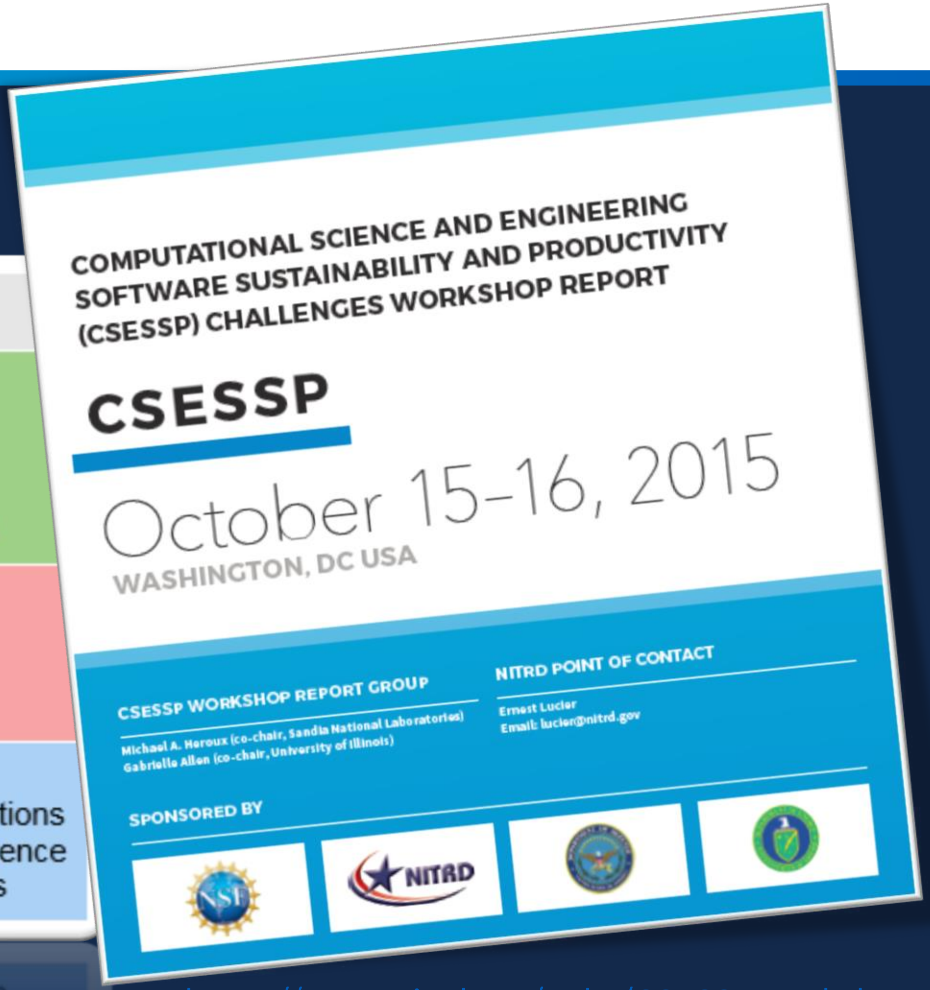
- Non-Ergodic (e.g., nucleation)
- Eigenfrequency (e.g., resonance)
- Discontinuity (e.g., phase transition)
- Stochasticity (e.g., turbulence)

Sparsity vs. Characterization Complexity

- Time/cost to generate synthetic data
- Time/cost to generate experimental data
- Consistency/Cost of data fusion between experimental + synthetic sources
- Dimensionality selection & hidden variables
- Access (proprietary and/or classification)
- Cost to validate synthetic data
- Cost to validate labeling of data

Challenge: Metrics and Incentives (financial recognition) / GAAP

	Engines of Productivity	Instruments for Insight
Increase	Return on Labor Profit Margins Supply Chain & Distribution Efficiency Design Exploration Agility to Seize Opportunities	Product Diversity & Novelty Yields & Production Capacity Data-driven decisions Trade-off Analysis Perception of Previously Unseen
Decrease	Costs of Overhead & Rework Time to Market Equipment Downtime Response Time to Fix Problems	Operational Exposure Uncertainty & Risk Contradictions Noise obscuring Main Effect
Methods of Practice	Automation of repetitive tasks/tests Faster than real time simulation/analysis Digitally replicate studied resources Concurrent studies on parallel system	Model unmeasurable effects Isolate effects in complex interactions Observe without physical interference "Big Data" analysis and synthesis



https://www.nitrd.gov/pubs/CSESSPWorkshopReport.pdf

Suggested candidate metrics as captured in Industry/Manufacturing chapter of CSESSP Report (October, 2015)
NITRD Computational Science and Engineering Software Sustainability and Productivity Challenges Workshop
National Science Foundation, Networking & Information Technology Research & Development, Dept. of Defense, Dept. of Energy

Challenge: Incentives (cross-silo recognition / “True Digital Thread”)

	Engines of Productivity	Instruments for Insight
Increase	Return on Labor Profit Margins Supply Chain & Distribution Efficiency Design Exploration Agility to Seize Opportunities	Product Diversity & Novelty Yields & Production Capacity Data-driven decisions Trade-off Analysis Perception of Previously Unseen
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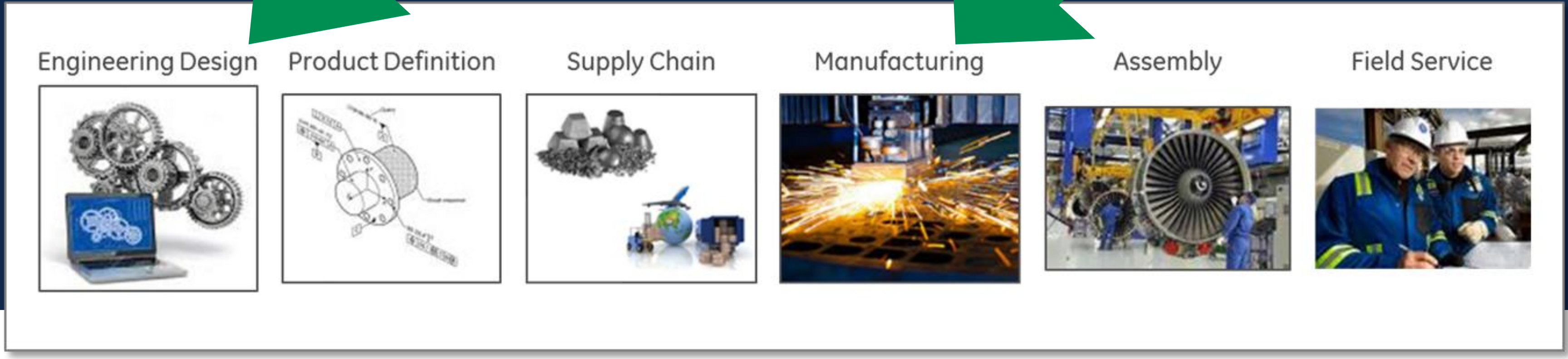
Even if metric is accepted – who gets the credit?

Organizational & Cultural Challenges

Cost Here

Payoff Here



Knowledge Challenge: Intellectual Debt

https://blog.usejournal.com/from-technical-debt-to-intellectual-debt-in-ai-e05ac56a502c

BEYOND EXPLAINABILITY: UNDERSTANDING

***Technical debt** arises when systems are tweaked hastily, catering to an immediate need to save money or implement a new feature, while increasing long-term complexity. […] When something stops working, this technical debt often needs to be paid down as an aggravating lump sum.*

Intellectual Debt: With Great Power Comes Great Ignorance

Jonathan Zittrain, Jul 24

This kind of discovery — ***answers first, explanations later*** — I call "intellectual debt."

We gain insight into what works without knowing why it works. We can put that insight to use immediately, and then tell ourselves we'll figure out the details later [debt to be paid in the future].

We are borrowing as a society, rather than individually; artificial intelligence and specifically, machine learning are [being applied] to a seemingly unlimited number of new areas of inquiry. The distinct promise of machine learning lies in suggesting answers to fuzzy, open-ended questions by identifying patterns and making predictions.

1. When we don't know how something works, it becomes hard to **predict** how well it will **adjust to unusual situations**.
2. Machine learning models are becoming pervasive, **compounding black box opacity**:
   a. oracular answers to single problems can generate consistently helpful results, but
   b. as AI systems gather and ingest data, they produce data of their own, then consumed by still other AI systems.
3. We need to know our exposure: we should invest in a **collective intellectual debt balance sheet**. We must keep track of just where we've plugged in the answers
4. Traditional debt shifts control: from borrower to lender, and from future to past, as later decisions are constrained by earlier bargains. Answers without theory — intellectual debt — also will shift control in subtle ways. […] A world of knowledge without understanding becomes, to those of us living in it, a world without discernible cause and effect, and thus a world where **we might become dependent on our own digital concierges** to tell us what to do and when.
5. Without the theory, we lose the autonomy that comes from **knowing what we don't know**.

Challenge: Foundational Limits of AI/ML

Opportunity: [Science of {AI/ML] for Science}

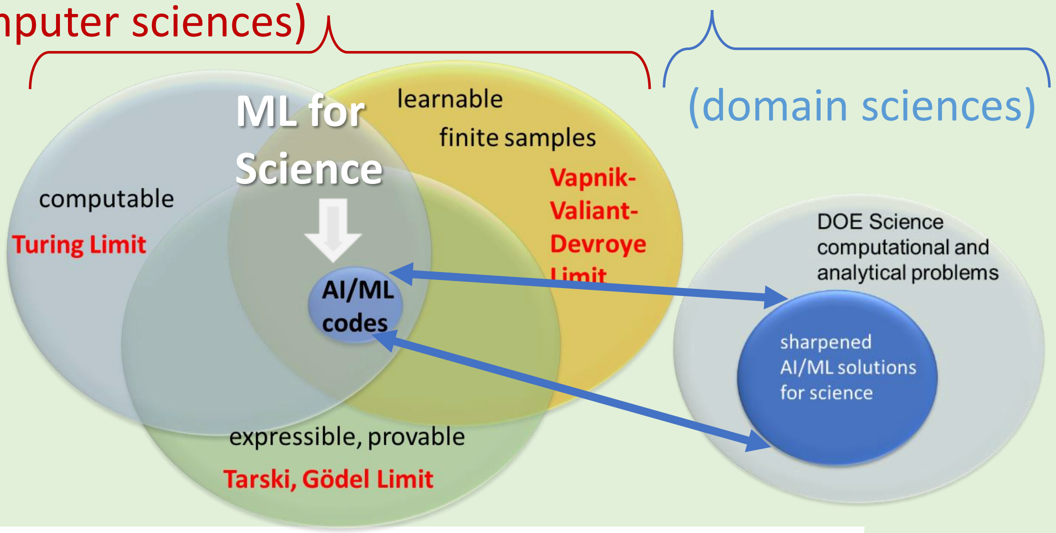
Credit: Nagi Rao
raons@ornl.gov

ML/AI methods do not solve all problems:

some are simply too complex for machines
- detection of zero-day computer viruses
- resilient codes to arbitrary hardware failures
- Inference of chaotic dynamics of TCP flows

AI/ML Solutions exploit underlying sciences
- ensure solvability: computable, learnable, expressible, provable
- sharpen AI/ML solutions: structure and constraints from laws

Science of AI/ML for Science



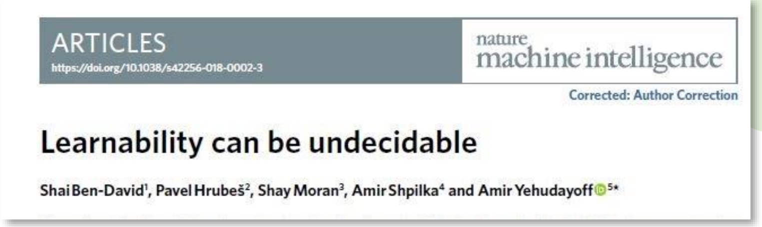
The reasoning is as follows: consider AI/ML method that attempts to discover laws (truths) from data as being attempted in several science areas. An explanation of truth is proof. But Gödel's theorem (a version) shows that we cannot mechanically provide proofs for all truths – so some truths will remain undiscovered by ML/AI method.

The implications could be quite deep: one can write ML codes that to try to solve this problem but its output would be either incomplete or unsound or both – if applied without care, this ML solution could potentially output "pseudo untrue" laws.

Not ML Solvable:

Classes of problems with properties at limits:

- ***Computability limit*** (undecidability)
  Church's proof that Hilbert's Entscheidungsproblem is unsolvable, and Turing's theorem that there is no algorithm to solve the halting problem.
- **Expressability limit** (cannot state into formalism)
  Tarski's undefinability theorem on the formal undefinability of truth
- ***Provability limit*** (Gödel's incompleteness theorems)


ARTICLES
https://doi.org/10.1038/s42256-018-0002-3
nature machine intelligence
Corrected: Author Correction

Learnability can be undecidable

Shai Ben-David[1], Pavel Hrubeš[2], Shay Moran[3], Amir Shpilka[4] and Amir Yehudayoff[5*]

- ***Learnability limit*** (can only resolve problem by choosing an axiomatic universe within which it is applicable therefore solution is not applicable to data outside that universe – i.e. sampling from separate infinities)
  (Vapnik <learnability> / Valiant <learnability-paper / PPT> / Devroye <A Probabilistic Theory of Pattern Recognition> - esp. slow rates of convergence – chapter 7)
  E.g., unbounded deviation from Bayes', infinite Vapnik-Chervonenkis dimension, …

(See also: Five Machine Learning Paradoxes that will Change the Way You Think About Data)

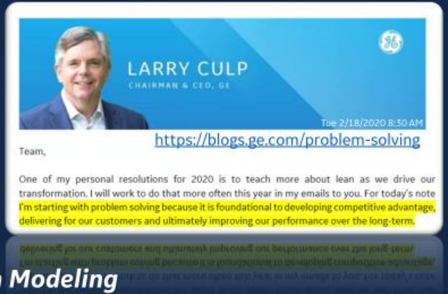
Physical-Abstract Hybrid Laws lead to sharpened AI/ML:
- Physical, abstract, hybrid laws
  - physical systems
  - cyber infrastructures
  - cyber-physical systems
- Customized AI/ML solutions may exploit
  - structure
    - relationships, correlations
  - constraints

Apply Characterization: Analytical and mathematical characterizations of limits and their interpretation within application/domain context

Summary

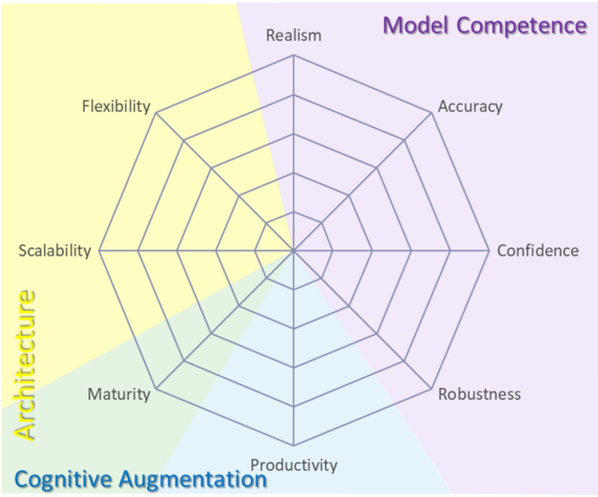
Criticality of Computational Methods, Model Maturity, Co-Design, Public-Private Engagement

Engineering's core competency
is **Problem Solving**



Problem Solving** critically relies upon **Modeling
(the problem, the solution and the process in between)

Modeling** critically relies upon **Computational Methods
(as an engine for scale, productivity, consistency and capability)



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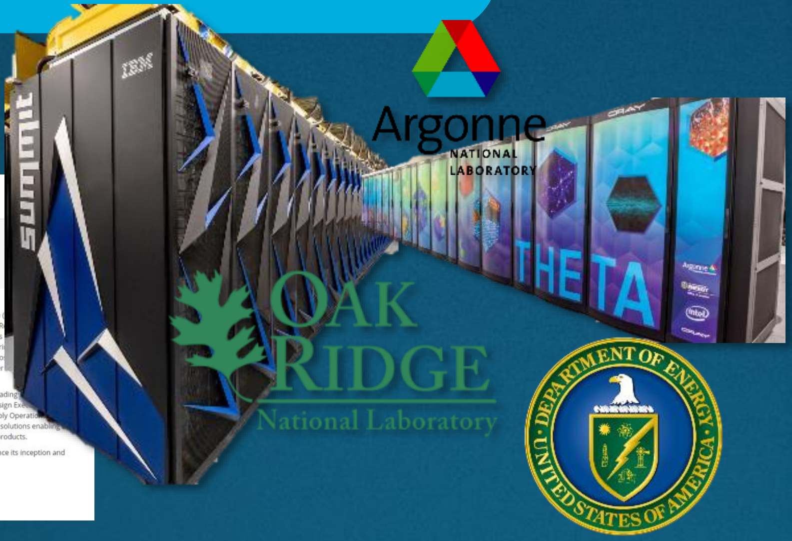
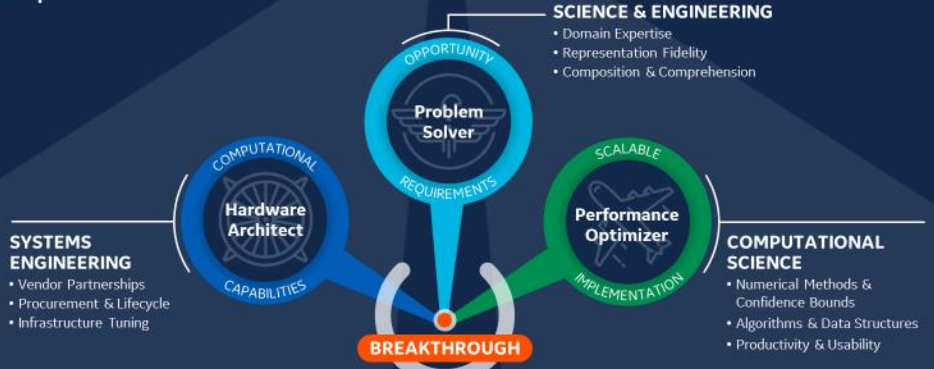
GE engagement with Government Leadership Computing

Exascale Computing Project
Industry Council Chair
GE Research CIO Dave Kepczynski

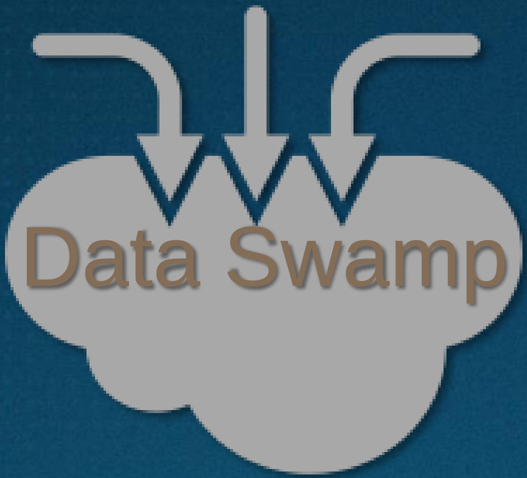


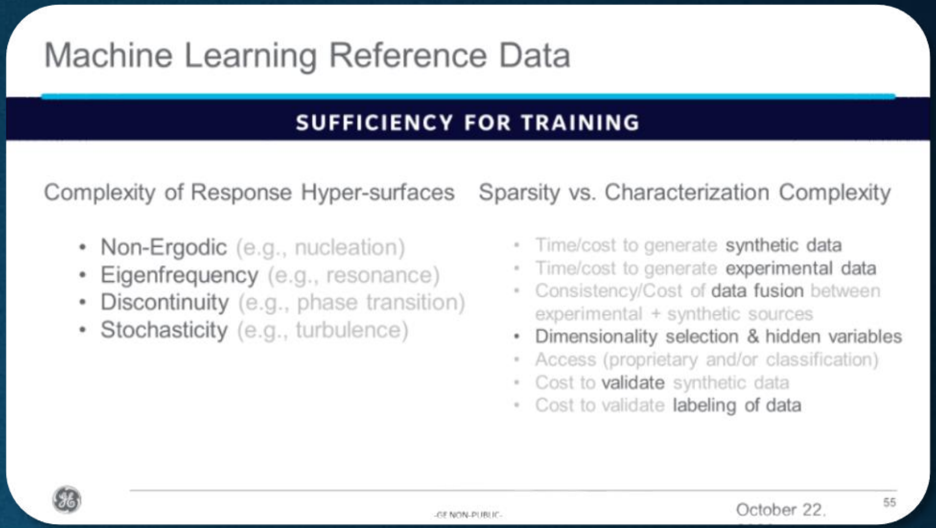
Co-Design: Landing Opportunities from Blue Sky Aspirations

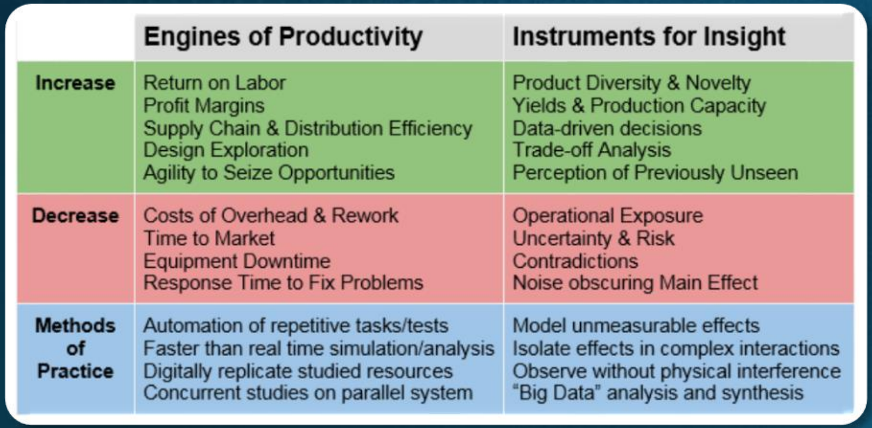


Challenges

Legacy







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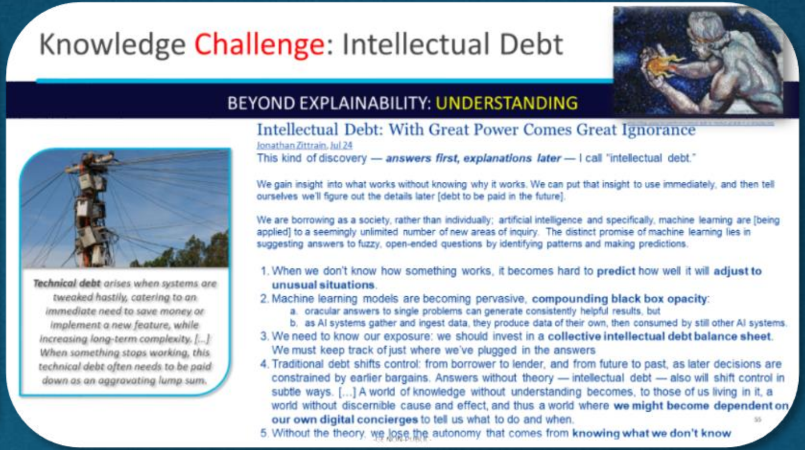

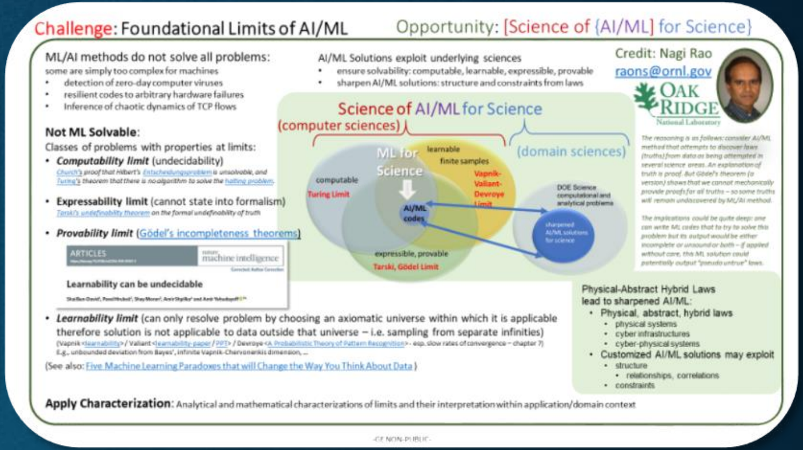

Metrics & Incentives