NS&T ML-AI

Big Data Machine Learning Artificial Intelligence

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Welcome to the

Artificial Intelligence and Machine Learning Symposium 5.0

June 8, 2021

IDAHO NATIONAL LABORATORY

NS&T ML-AI

Big Data   Machine Learning   Artificial Intelligence

Welcome

Ronald Boring, PhD, FHFES

Manager, Human Factors and Reliability Department

INL

Craig Primer, Light Water Reactor Sustainability
Nuclear Safety and Regulatory Research Division
Idaho National Laboratory

Machine Learning & Artificial Intelligence Symposium 5.0

Tuesday, June 8, 2021

Moving from 2020 to 2021 - Symposium 5.0

- Last year INL sponsored quarterly symposiums on Artificial Intelligence (AI) and Machine Learning (ML) approaches and activities related to science and engineering
  - The “1.0 Symposium” focused on internal-to-INL activities and capabilities
  - Symposium 2.0 we broadened the focus and highlighted activities and capabilities around the nuclear industry and universities
  - Symposium 3.0, we invited researchers provide updates on nuclear-related applications using AI/ML
  - Symposium 4.0, introduced the concept of "Trustworthy" as it relates to AI/ML
- We continue our discussion today on the importance of Trustworthy AI/ML development and hear from researchers about their work in these areas

Presenters and Topics

11:00 (MDT)	**Welcome, Introduction, and Agenda**	**Craig Primer, INL**
11:05	Machine Learning Pillars to Avoid Embarrassment for Trustworthy and Explainable ML	**Rita Foster, INL** **Andrea Mack, INL** **Shaya Wolf, UofWY**
11:35	Large-scale Optimization of Boiling Water Reactor Bundles with Hybrid Reinforcement Learning and Evolutionary Intelligence	**Majdi Radaideh, MIT**
11:45	Robust data-driven sensor placement	**Krithika Manohar, UW**
11:55	Cyber-Physical State Awareness, Automated Response and Confirmed Resilience	**Craig Rieger, INL**
12:05	Human-Centered Artificial Intelligence	**Ben Shneiderman, UMD**
12:35	Designing Explainable AI	**Torrey Mortenson, INL**
12:45	Explainable Dimensionality Reduction Using Scientific Constraints	**Ramakrishnan (Ramki) Kannan, ORNL**
12:55	**Closing Remarks**	**Craig Primer, INL**

Idaho National Laboratory

Rita Foster, Andrea Mack, Shaya Wolf

Infrastructure Security

Pillars to Avoid Embarrassment for Trustworthy & Explainable ML

Trustworthy AI/ML Symposium

June 8, 2021

Idaho National Laboratory

Agenda

- Background
- ML/Graph Pillars
  - Purpose
  - Relevance
  - Data Types
  - Data Sources
  - Data Management ***and more data***
  - Data Validation
  - Explainable
  - Trustworthy

Why it is relevant to ML/AI Future

- Why ML Pillars ?
  - Layers of validated assumptions for purpose, relevance, data and ML concepts
  - Provide improvement, feedback to challenge all concepts
  - Assist in explaining ML concepts to potential sponsors
    - Enable refinement to match sponsor’s needs
    - Gain critical partnerships based on problem, data and ML relevance
- Our experience with test corpora concepts enable multi-faceted analysis
  - Benefits of rapid prototyping of new ML/AI methods
  - Actionable ML results from Agile data sets
  - Higher fidelity analysis with ability to challenge assumptions and results

Good research yields more questions enabling future research questions

Machine Learning for Cyber Protection Critical Infrastructure

Historical Journey

Reverse Engineered Binaries

2017 - 2021

DOE-CESER
Firmware Indicator Translation (FIT) – implemented 2 LDRD methods from RE@Scale

2020 - 2023

Grid Modernization Laboratory Call – **Firmware Command and Control (FC2)**

Structured Threat

2019 - 2022

DOE-CESER Competitive Laboratory Call

Geo Threat Observable (GTO)

Malware

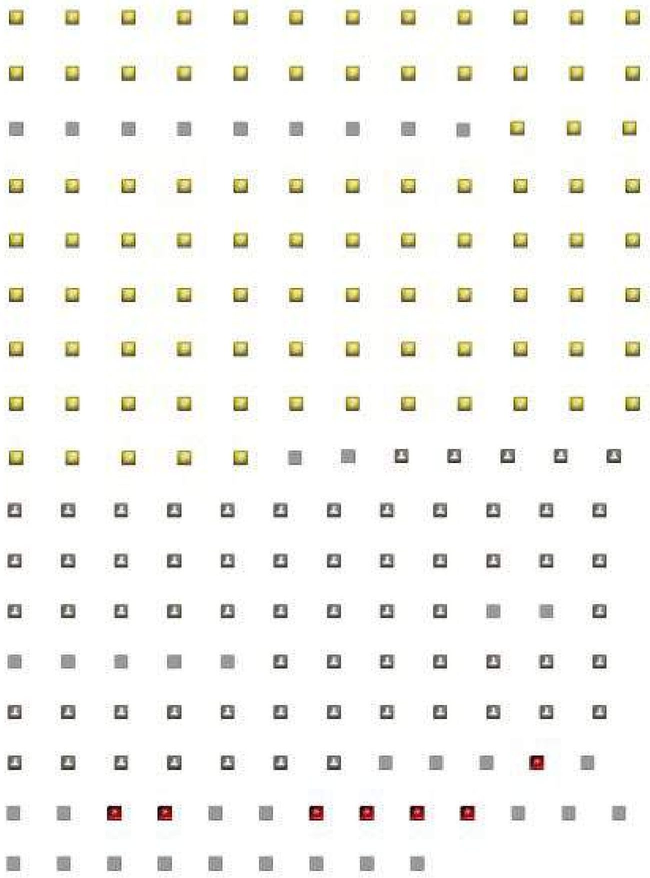
2020 - 2023

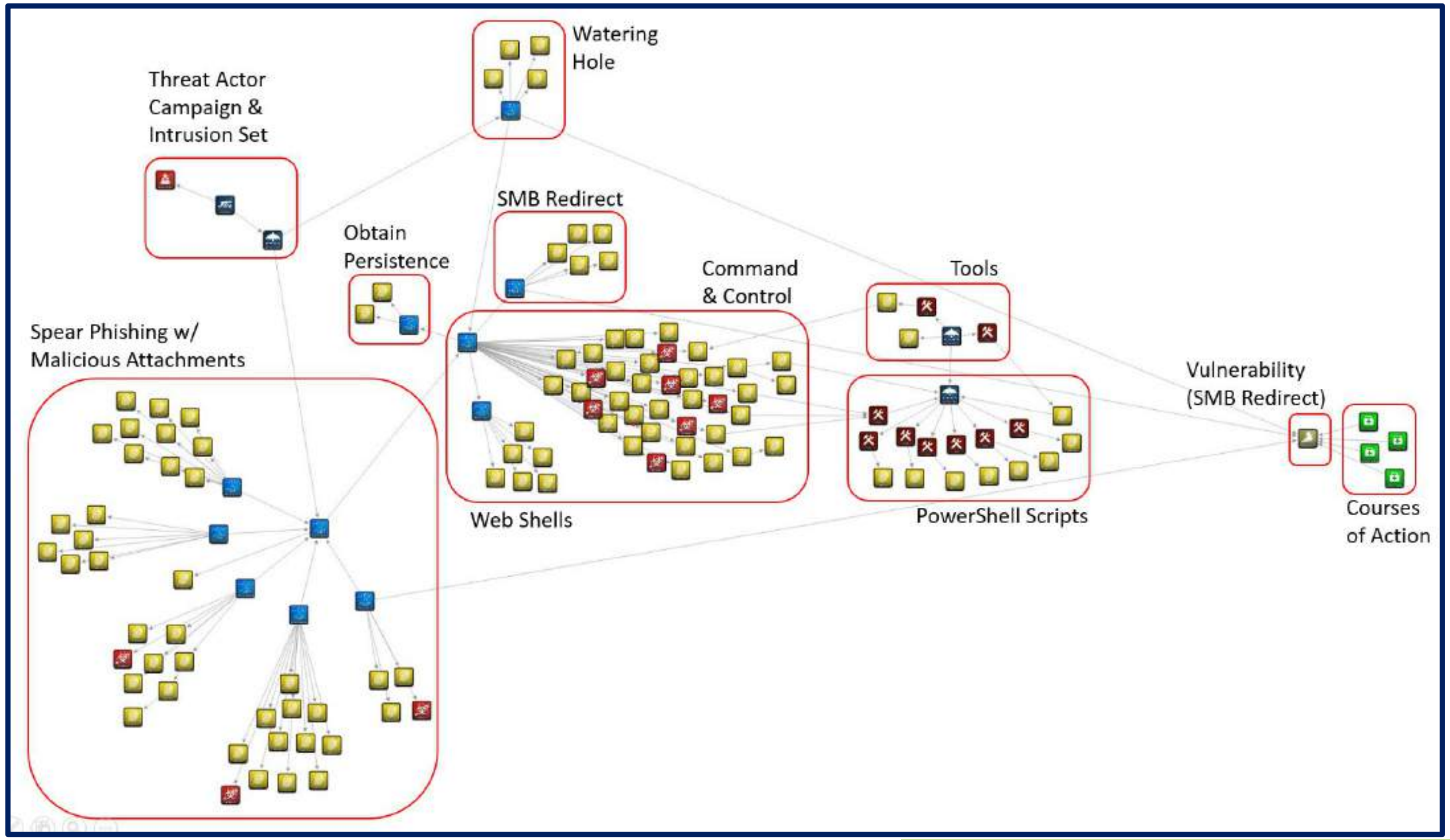
Grid Modernization Laboratory Call – **Deep Learning Malware (DLM)**

Case Study 1 – Structure Threat - Explainable

ML Pillars	Structured Threat
Explainable	STIG

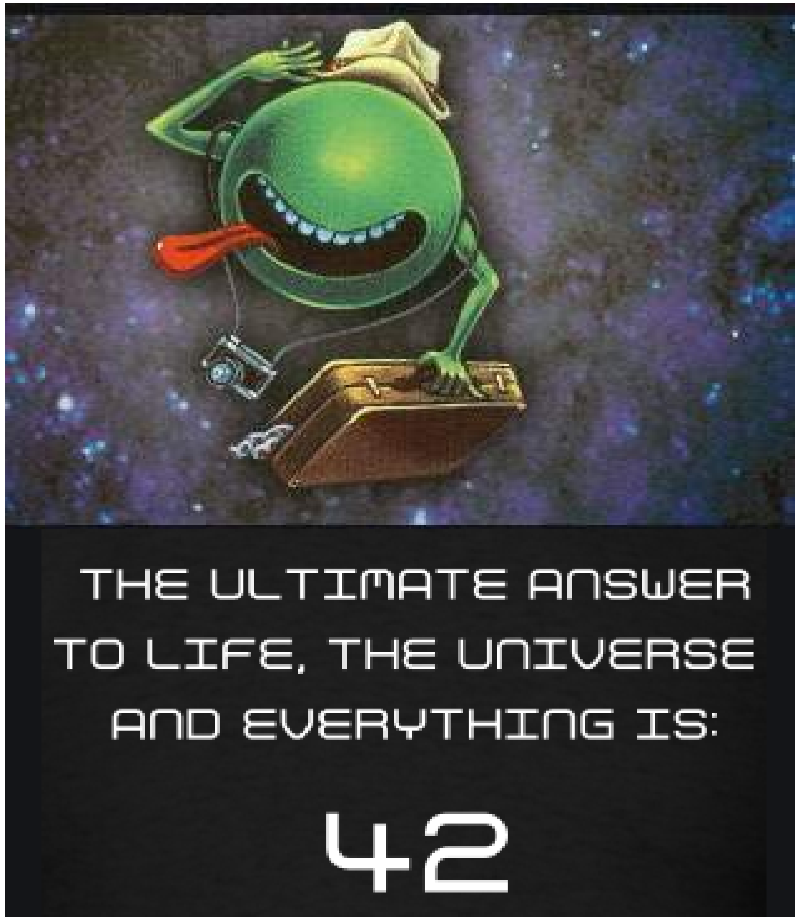
STIG
Structured Threat Intelligence Graph

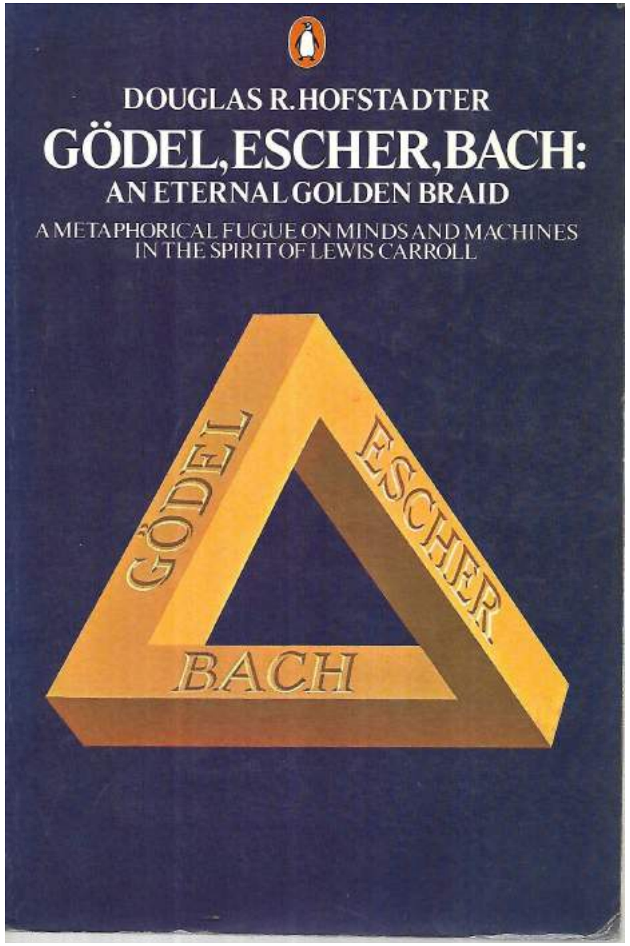




Russians in the Grid Example – Bryan Beckman

Machine Learning Explainable & Trustworthy Spectrum

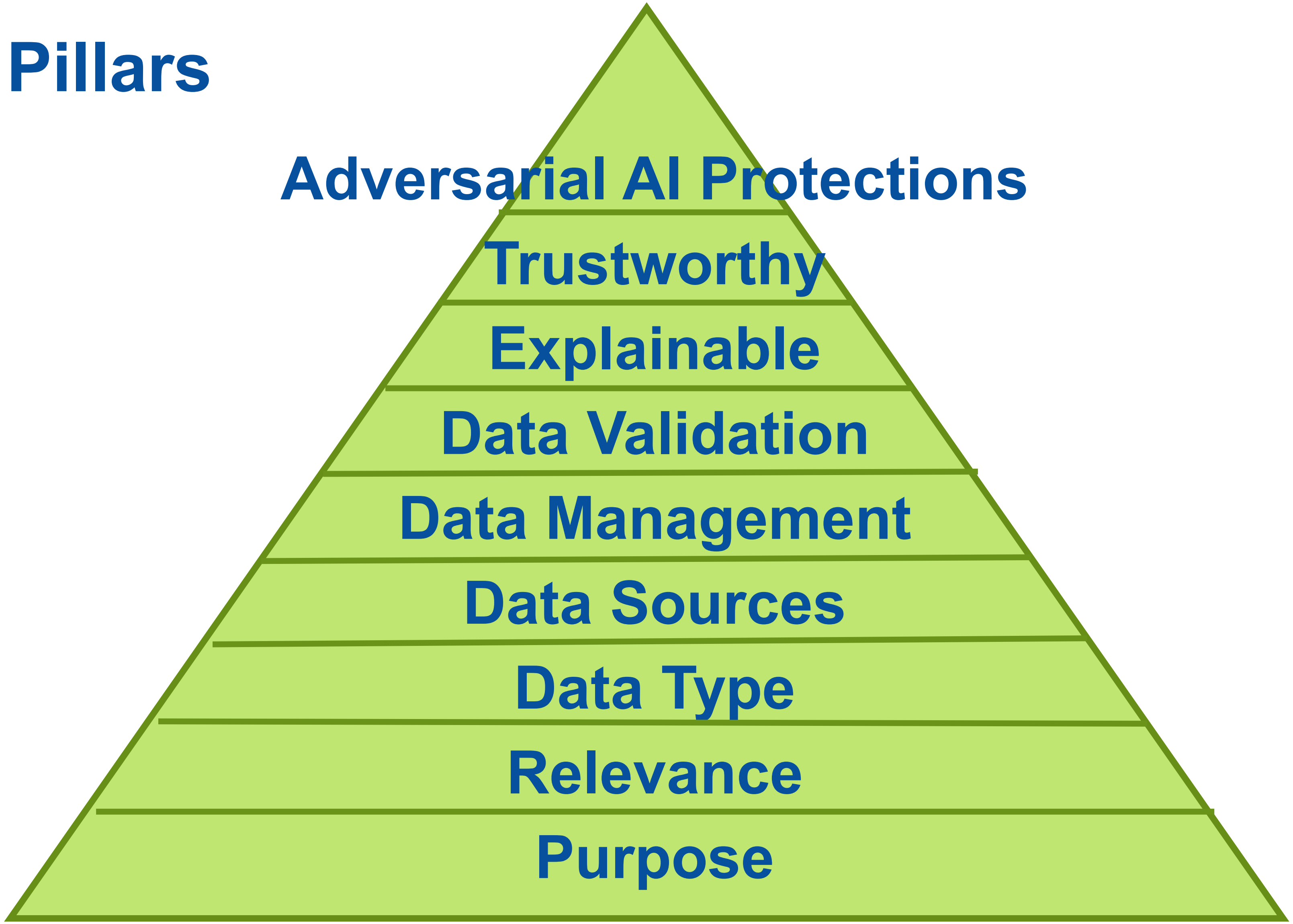




Essential Abilities for Intelligence

- Flexibility - Respond to situations Take advantage of fortuitous circumstances;
- Make sense out of ambiguous or contradictory messages;
- Recognize the relative importance of different elements of a situations;
- Find similarities between situations despite differences which may separate;
- Draw distinctions between situations despite similarities which may link;
- Synthesize new concepts by taking old concepts and putting together in new ways;
- Generate novel concepts and ideas

ML Concept Pillars



Case Study 1 – Structure Threat - Purpose

ML Pillars	Structured Threat
Purpose	GTO will connect missing cyber threat links and provide prediction, mapping to situational awareness for impact, threat analysis and ad-hoc scenarios enabling better use of limited cyber defense resources.

Goal and Objectives

- Goal: Provide common operational picture for cyber defenders to stage limited resources
- Leverage visualization mechanisms for GIS
- Define structured threat to GIS layers for visualization
- …

Capabilities/Gap Analysis

	Cost	Sharable	Actionable	
CYBER THREAT ALLIANCE	Free	Yes	Yes	Contex Data
Argonne NATIONAL LABORATORY (Cyber Fed Model)	Free	Yes	Yes	No
AIS Automated Indicator Sharing	Free	Yes	No	No
HOPLITE INDUSTRIES	Paid	No	Yes	Unkno
MISP Threat Sharing	Free	Yes	Yes	Genera Snort, Y etc.
ALIEN VAULT	Free	Yes (Two Way)	Yes	IOC Depend
CVE NVD	Free	Yes	No	JSON
CRISP	Free			

Potential Outcomes

- Interactive GIS display of current and evolving threat
- Test corpora …machine learning of similarities to past and predict evolving
- Ad-hoc scenario capability…for Machine Leaning threat behavior
- …

Scope definition

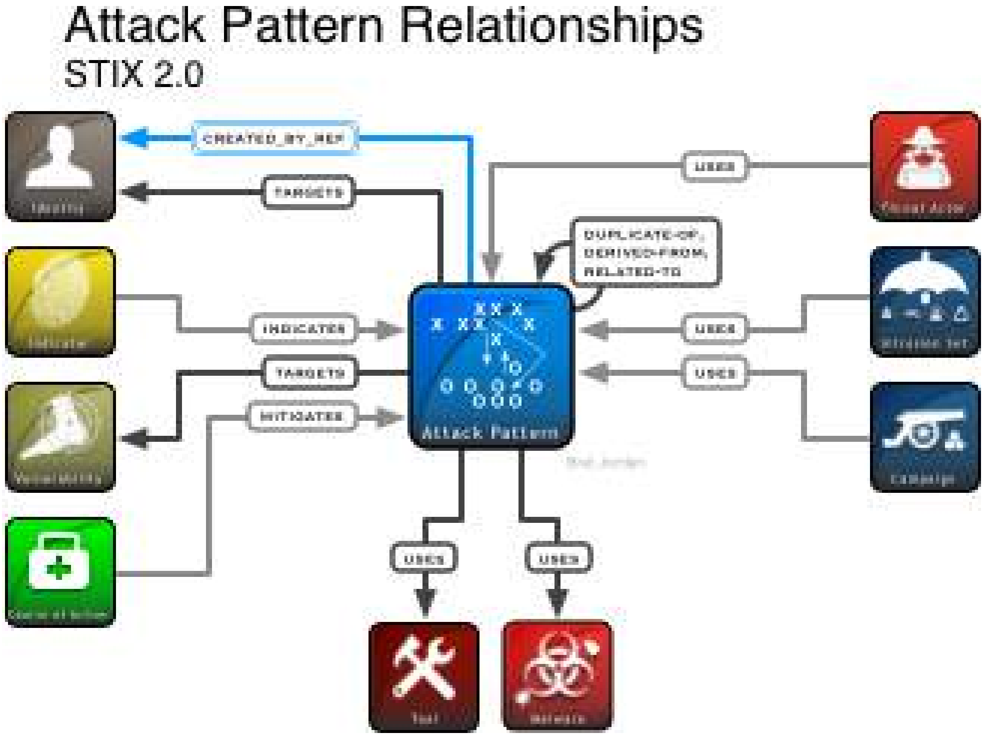
ML/AI Appropriateness origin and accounting for uncertainty

Case Study 1 – Structure Threat - Relevance

ML Pillars	Structured Threat
Relevance	STIX

Structured Threat Information Expression

- International Standard Open Source
- OASIS Standard
- Hundreds of Users
- Active Standard being Enriched
- Large use enables technology adoption
- STIX has proven to be **Sharable, Actionable** and **Implementable**
- Relevance for Critical Cost Share Partners: Splunk, Forescout, FortiNet, Eclypsium, Asset Owners, and many original equipment manufacturers



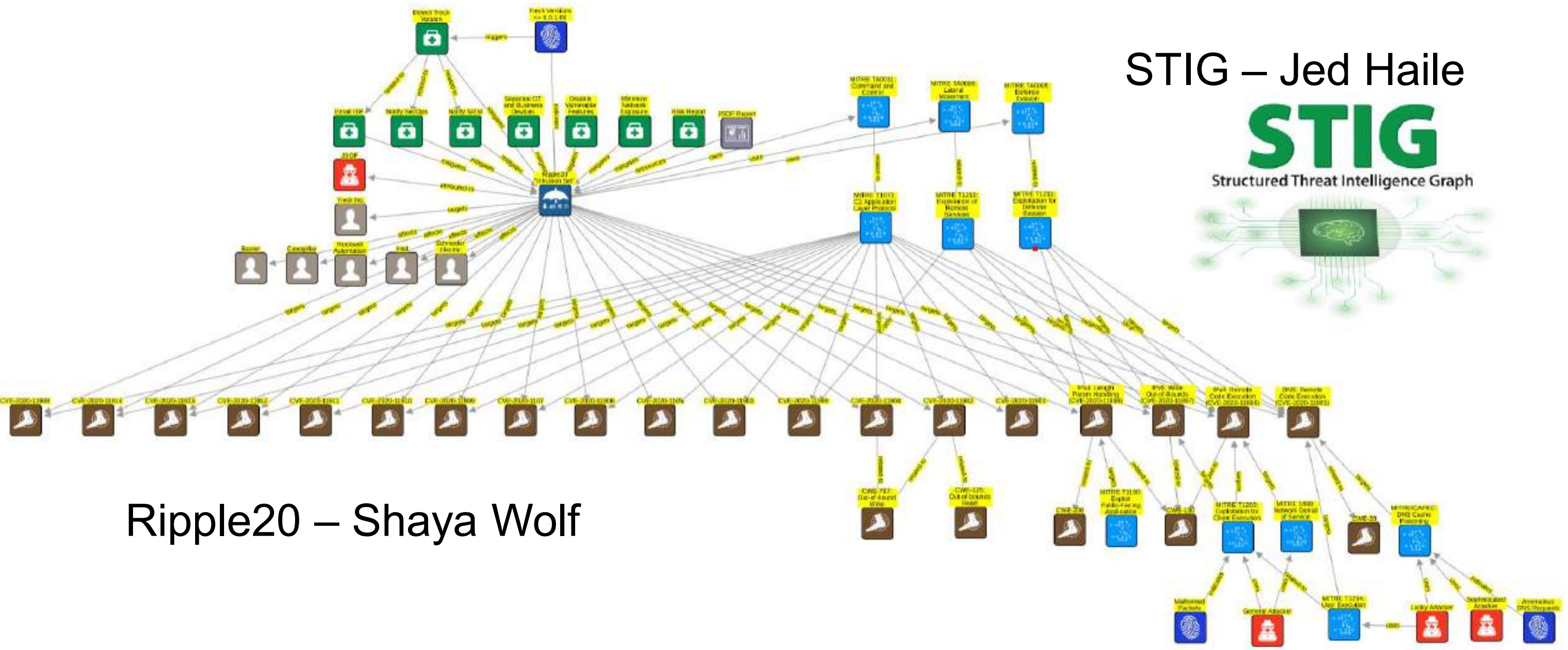
Case Study 1 – Structure Threat – Data Type & Sources

ML Pillars	Structured Threat
Data Type	Structured Threat in Graph database
Data Sources	Threat Feeds; Scraped, Enriched

STIG – Jed Haile

STIG

Structured Threat Intelligence Graph



Ripple20 – Shaya Wolf

ATT&CK®

VIRUSTOTAL

MISP Threat Sharing

NVD

CVE Common Vulnerabilities and Exposure

CWE

NIST Information Technology Laboratory NATIONAL VULNERABILITY DATABASE

Case Study 1 – Structure Threat – Managed & Validation

ML Pillars	Structured Threat
Data Managed	Graph Database
Data Validation	Nodal Analysis

Node Analysis Andrea Mack

Graph Databases for Management:

- Edges, Nodes, Properties
- Graph Traversal – Simple: vertices/edges, Breath or Deep First Search

Structure - Feature generation using iGraph

- Communities within graphs;
- Degree of the graph;
- Cliques mean/max clique lengths
- Global Transitivity

Deeper context rich narratives

- Descriptions, evidence-based sources

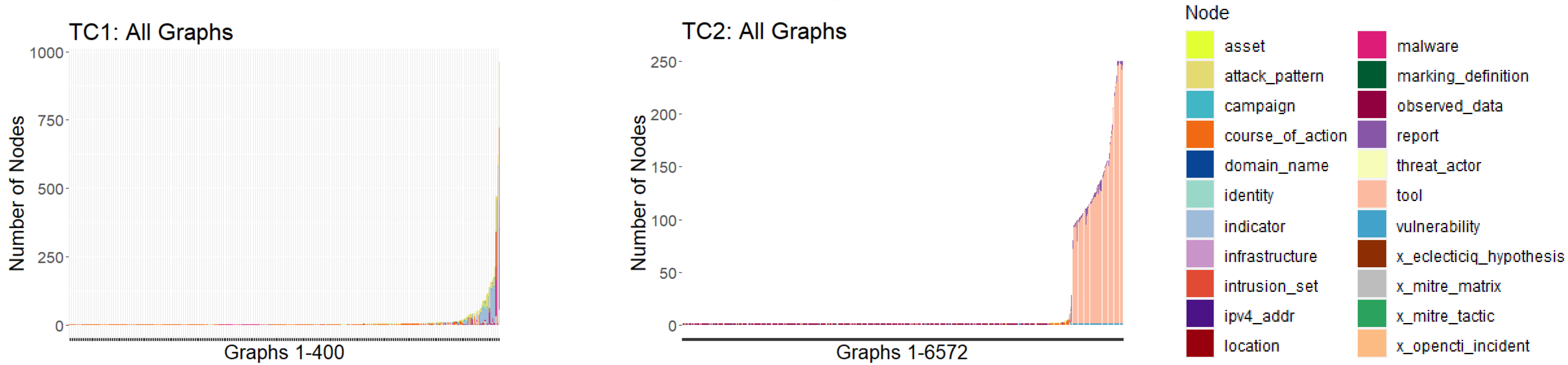
Nodal Analysis for Validation of Assumptions

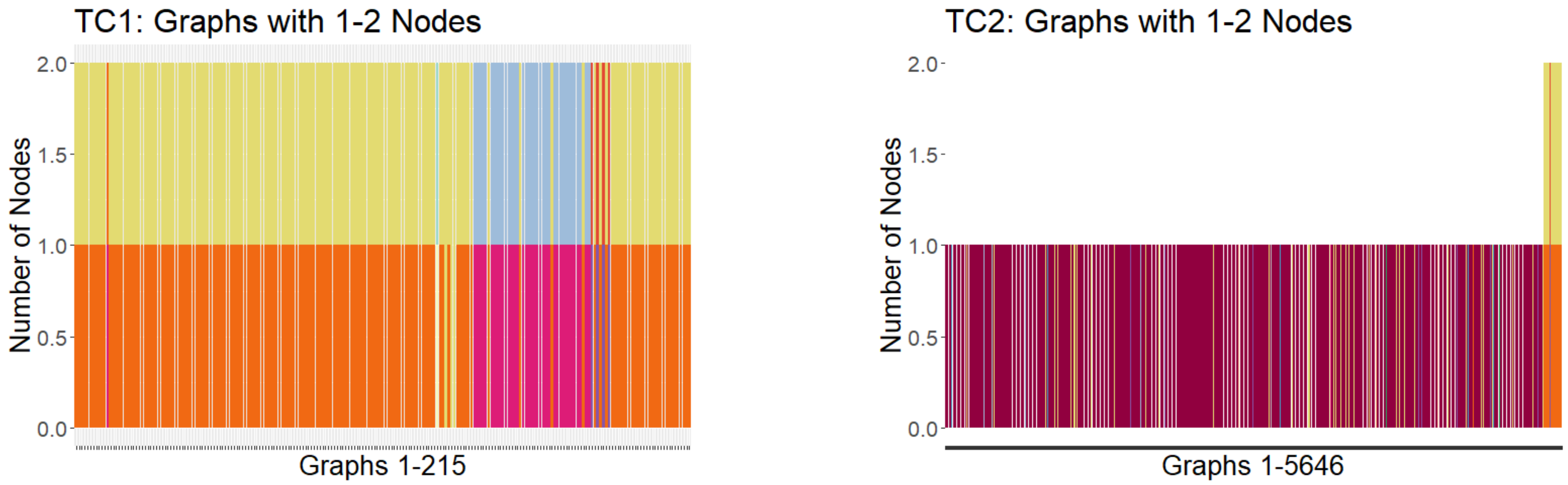
- Validate Test Corpora
- Validate Data Assumptions
  - Subject Matter Expert Review
- Repeatable Embeddings for ML – Graph CNN to Persistent Homology

  i.e., Feature Vector count validated by simple Graph Queries

Nodal Analysis – Validation of Assumptions

What are the Context of All and Two node graphs?





Validation of Graph Context

Challenging the Value of one node graphs

Nodal Analysis

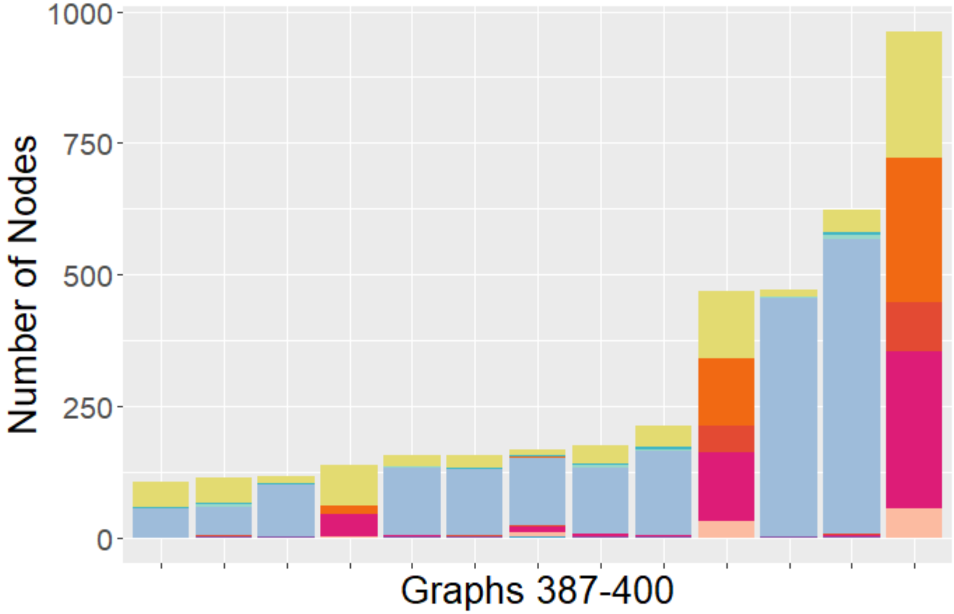
Over 100 Node Graph Analysis

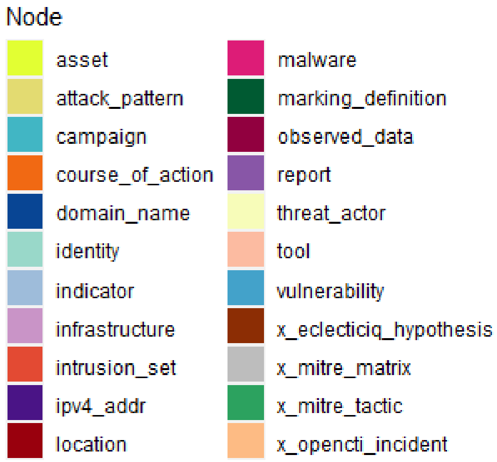
Nodes	TC1: Graphs	TC2: Graphs
1-2	215 (53.7%)	5646 (85.9%)
3-10	134 (33.5%)	131 (1.99%)
11-50	29 (7.25%)	42 (.6%)
51-100	9 (2.25%)	95 (1.45%)
101-max	13 (3.25%)	658 (10.0%)
Total	400	6572

Validation of Graph Context > 100 Nodes

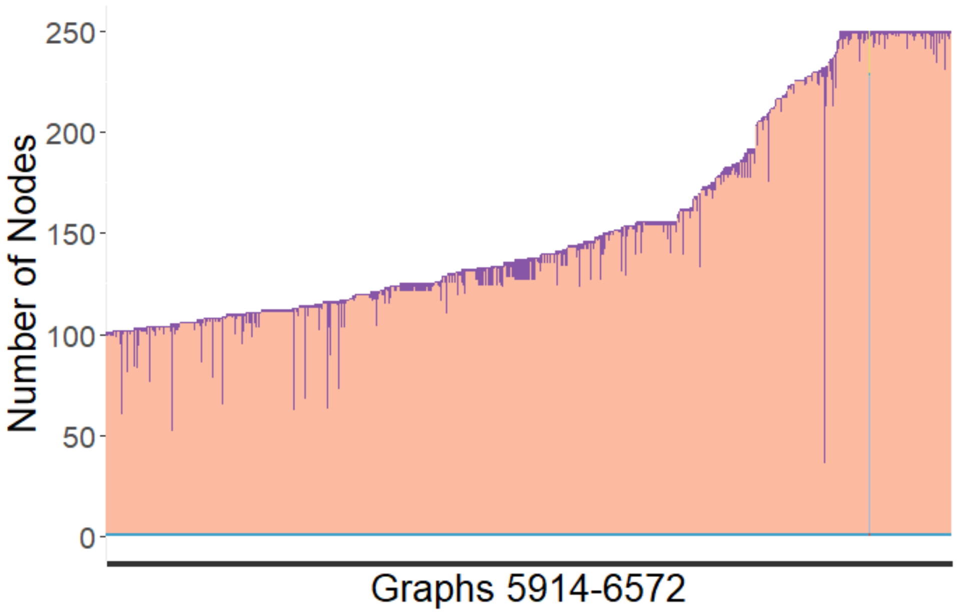
13 static vs 658 Enriched Graphs with more tools, behaviors

TC1: Graphs with > 100 Nodes





TC2: Graphs with > 100 Nodes

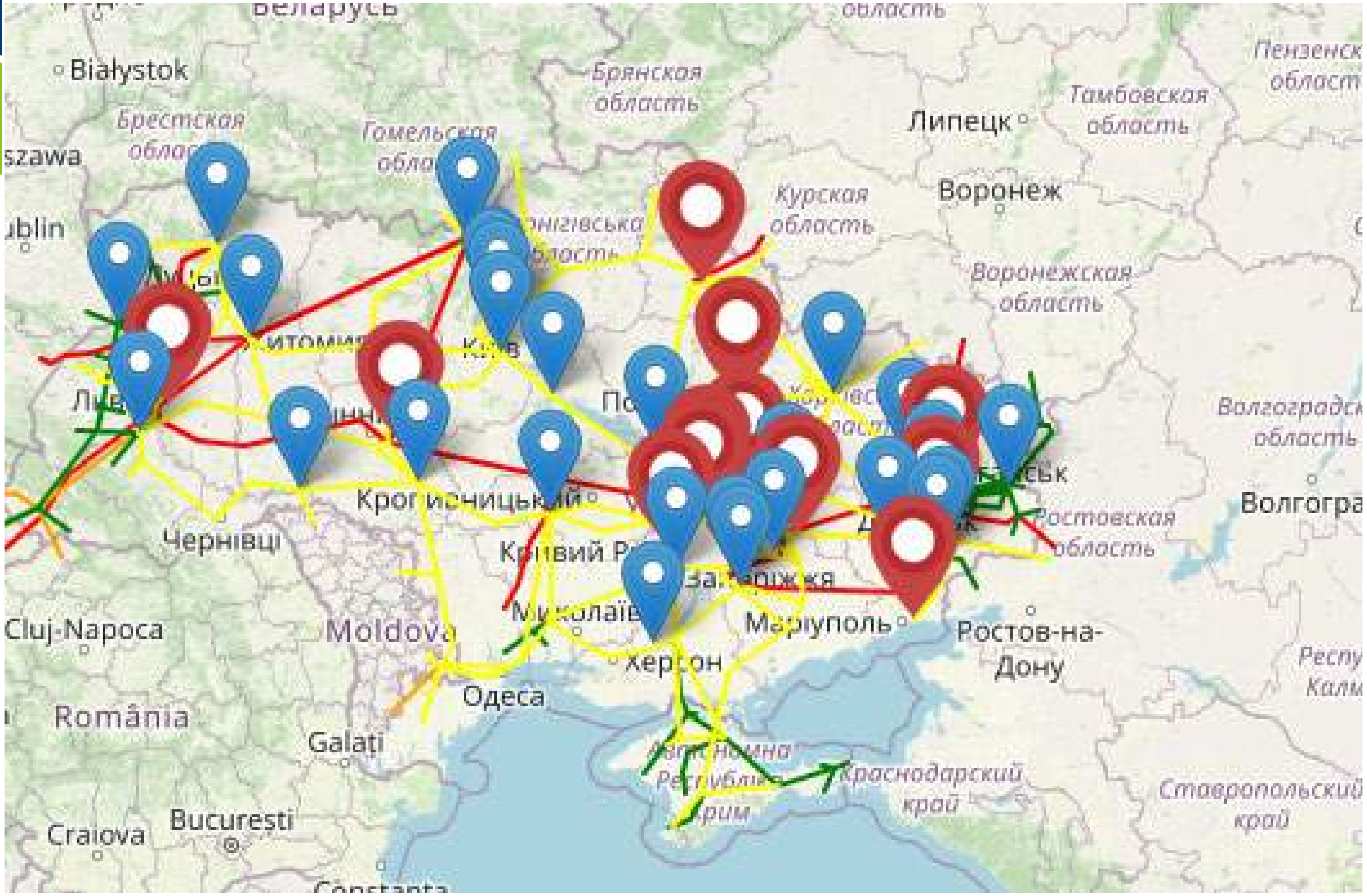


Case Study 1 – Structure Threat - Explainable

ML Pillars	Structured Threat
Explainable	Geo Threat Observable

Visualization

- Location of Cyber Attack
  - Kiev, Ukraine December 2016
- Electric Infrastructure Layers
- GIS
- Redrawn impact areas after ad-hoc scenarios; enhanced threat and prediction

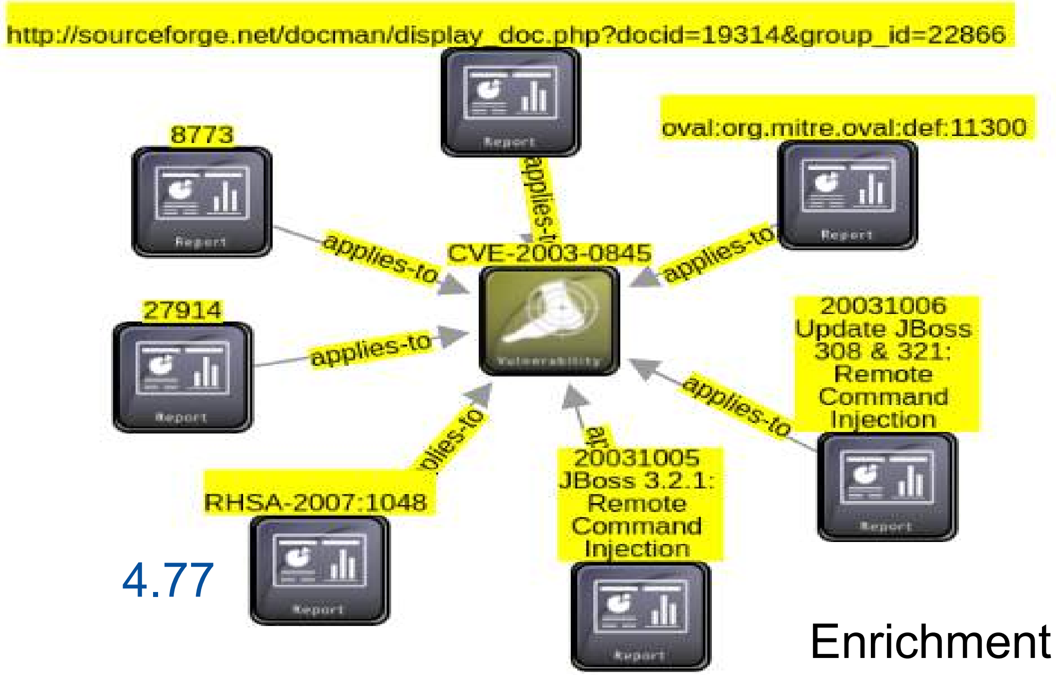


Kiev, Ukraine– Ryan Hruska

Case Study 1 – Structure Threat - Trustworthy

ML Pillars	Structured Threat
Trustworthy	Sources, Notes, Observables & Scoring

Evidence-Based Threat: Sources, Reports, Cyber Observables and Scoring to Trend Threat Value; Provides Feedback



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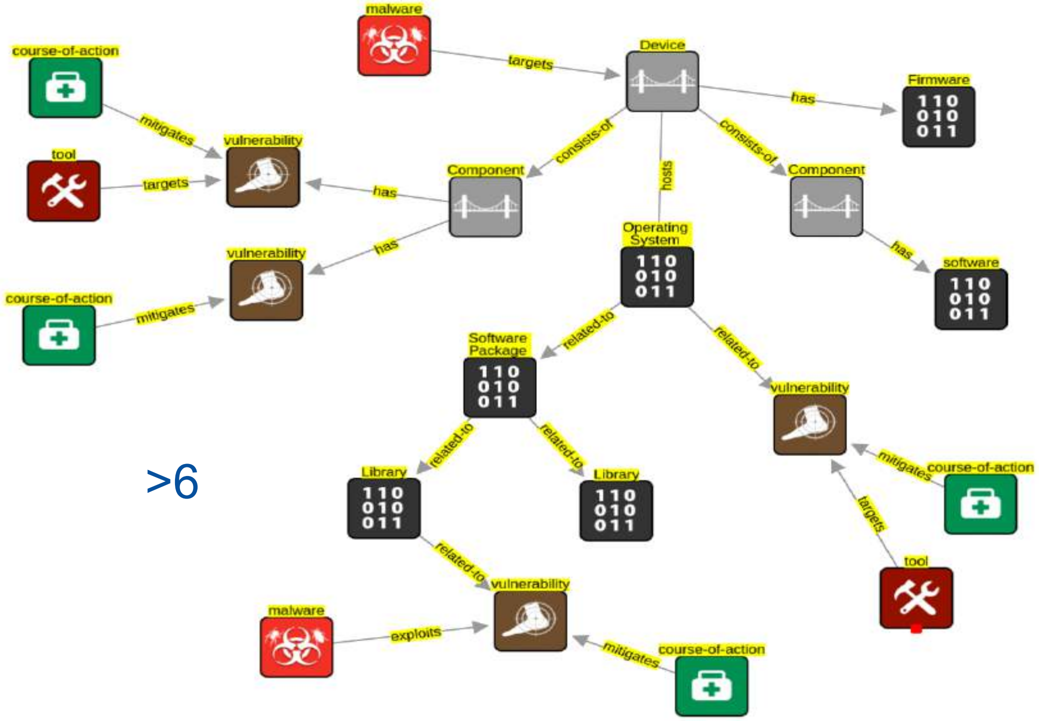


1.36

Enrichment Scoring – Bryan Beckman

Case Study 1 – Structure Threat - Trustworthy

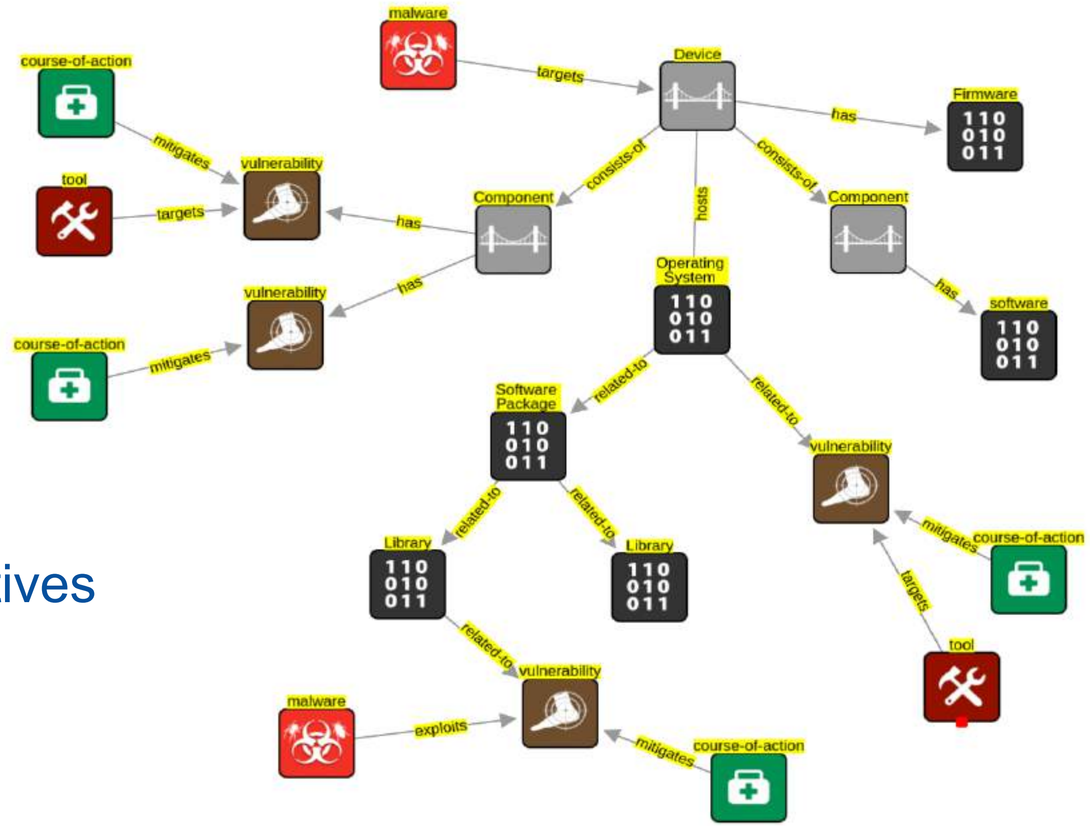
ML Pillars	Structured Threat
Trustworthy	Sources, Notes, Observables & Scoring

Process for Trustworthy

- Baseline Test Corpora
- Baseline Embeddings for ML
- Validate Baselines
- Trend Quality Scores
- Accuracy, repeatability, False Positives, False Negatives (F1)
- Feedback for enhancements and improvements
- Ability to Challenge Results

And Above All …

Curiosity



Attack Surface – Bryce McClurg

Looking Ahead

Continued use of ML Pillars

- Refined by external ML experts, research partners and included in strategy
- Focus concepts for future sponsors and stakeholders
- Relevance and actionable results
- Higher fidelity data understanding with visualizations for explainable basis
- Enabling feedback and ability to challenge concepts for improvement

- Test Corpora
  - Easier scope discussions – next iteration tasking
  - Repeatable embeddings with further analysis and validation
  - Two large test corpora Structured Threat and Translated Binaries

Future: critical infrastructure cyber protection issues

Questions?

Idaho National Laboratory

Majdi I. Radaideh
MIT Nuclear Science and Engineering

Large-scale Optimisation of BWR Bundles with Hybrid Reinforcement Learning and Evolutionary Intelligence

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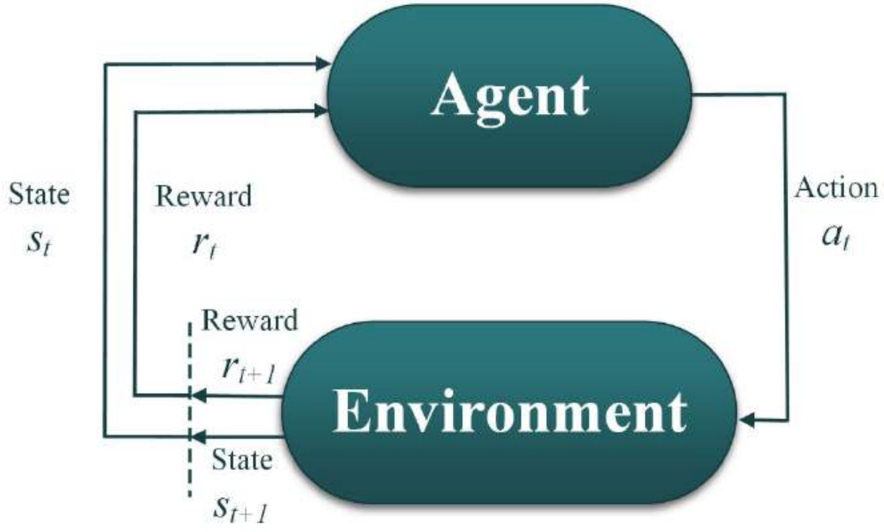
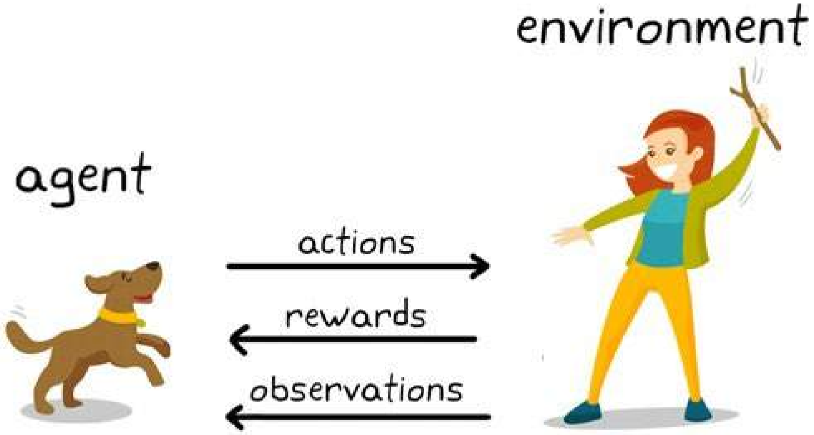
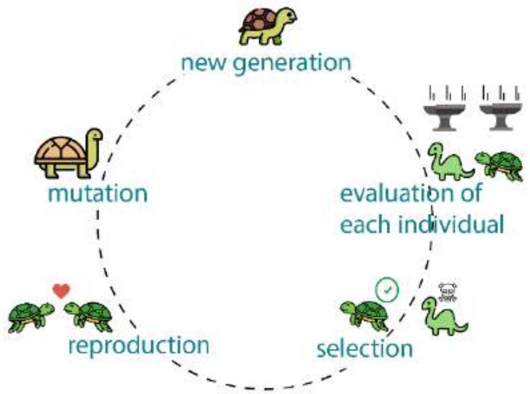
Reinforcement Learning & Evolutionary Computation

Reinforcement Learning



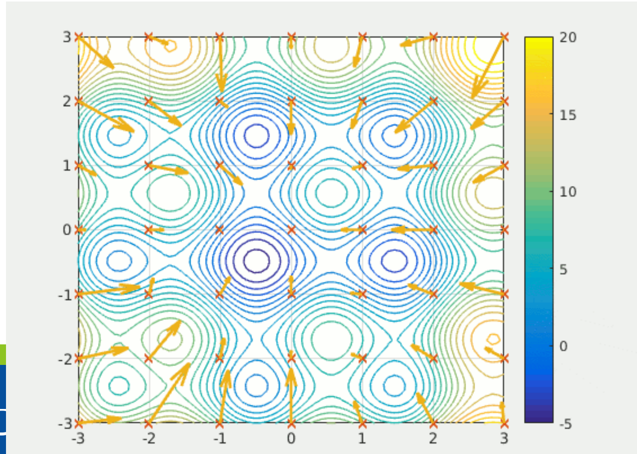


Genetic Algorithms



Grey wolf Optimization

Particle Swarm Optimization



Game-playing AI

I am almost there ☺

Why AI/ML for Fuel Optimization

- **Expensive** (fuel depletion is included and a bigger assembly is optimized GE14-10x10).
- **Combinatorial** (dicrete input space)
- **High-dimensional** (~10^{65} possibilities in the space)
- **Heavily-constrained** (43 constraints)
- **Multi-objective** (maximize burnup, minimize peaking factor)

$$\min_{\vec{x}} f(\vec{x}) = -\left[\frac{1}{3}\sum_{i=1}^{3} B^{z_i} - 10\max(PPF^{z_1}_{0\%}, ..., PPF^{z_3}_{0\%}, PPF^{z_1}_{40\%}, ..., PPF^{z_3}_{40\%}, PPF^{z_1}_{70\%}, ..., PPF^{z_3}_{70\%})\right], \quad (29)$$

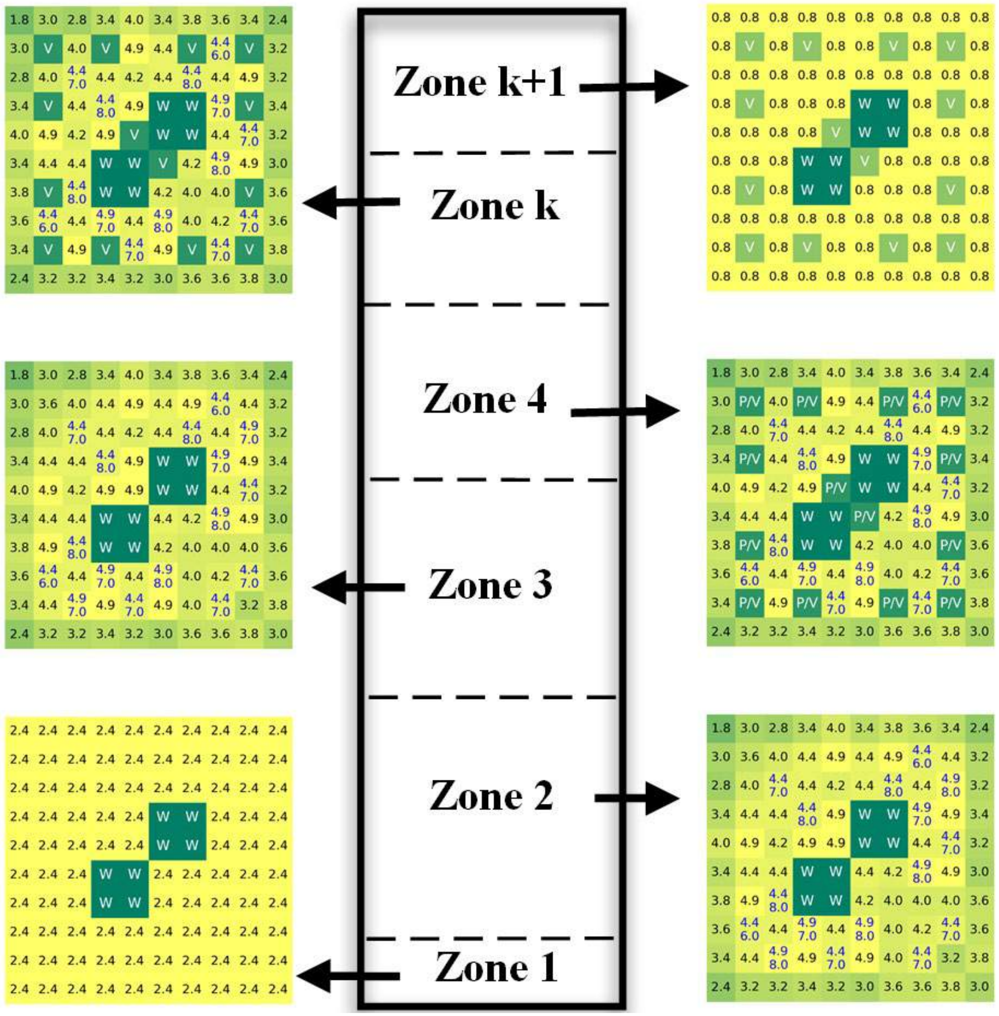
subject to the following constraints

$$g_1(\vec{x}) = 16 \leq N^{z_1}_{poison} \leq 18, \quad g_2(\vec{x}) = 16 \leq N^{z_2}_{poison} \leq 18, \quad g_3(\vec{x}) = 13 \leq N^{z_3}_{poison} \leq 16, \quad (30)$$

$$g_4(\vec{x}) = PPF^{z_1}_{0\%} \leq 1.45, \quad g_5(\vec{x}) = PPF^{z_2}_{0\%} \leq 1.45, \quad g_6(\vec{x}) = PPF^{z_3}_{0\%} \leq 1.45, \quad (31)$$

$$g_7(\vec{x}) = PPF^{z_1}_{40\%} \leq 1.4, \quad g_8(\vec{x}) = PPF^{z_2}_{40\%} \leq 1.4, \quad g_9(\vec{x}) = PPF^{z_3}_{40\%} \leq 1.4, \quad (32)$$

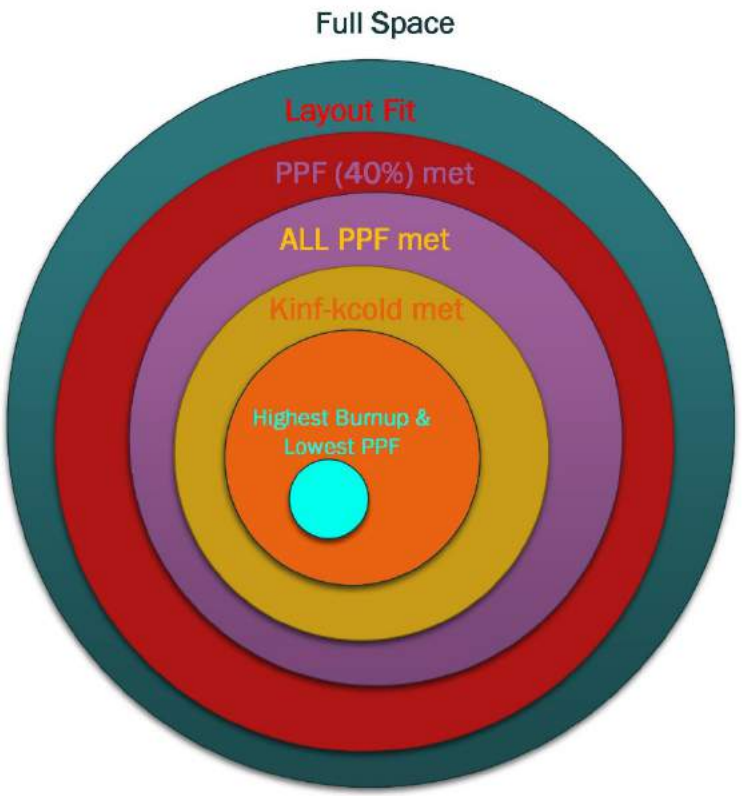
And many more!



Radaideh, M. I., Forget, B., Shirvan, K. (2021). Large-scale design optimisation of boiling water reactor bundles with neuroevolution. *Annals of Nuclear Energy*, *160*, 108355.

Divide-and-Conquer

- Step 1: Layout matchup
  - E, G, N_{gad}, GAD Positioning
- Step 2: PPF (40%) met (each CASMO case is 1.5s)
  - For all axial zones (PSZ, DOM, VAN1, VAN2)
- Step 3: ALL PPF are met (each CASMO case is 8s)
  - For all axial zones (PSZ, DOM, VAN1, VAN2)
  - For 0%, 40%, 70% void
  - For Rodded/Unrodded conditions
- Step 4: deplete the bundle and get k_{cold}/k_{hot} (each CASMO case is 2 min)
  - For all axial zones (PSZ, DOM, VAN1, VAN2)
- Step 5: Search for the best burnup & Lowest PPF



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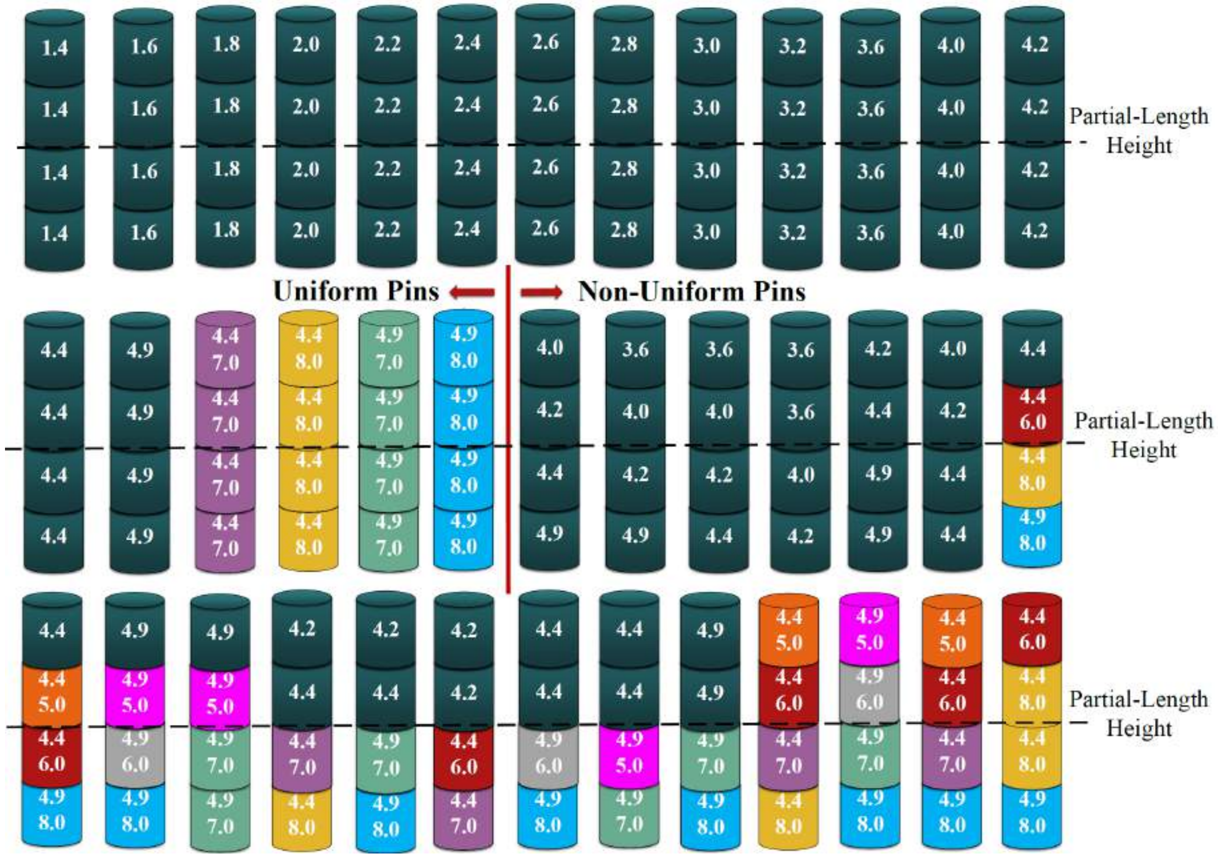
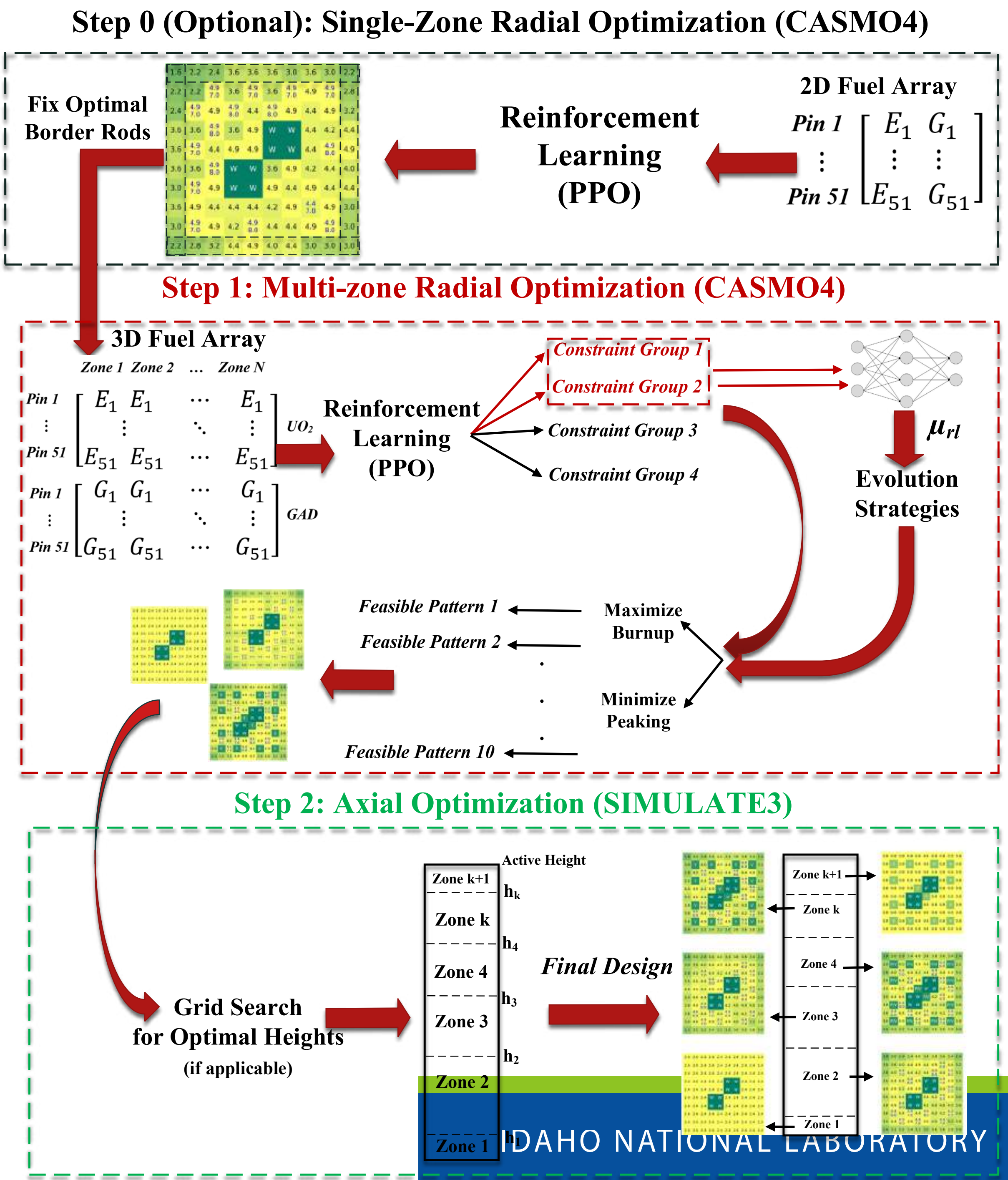
Large-scale Optimization





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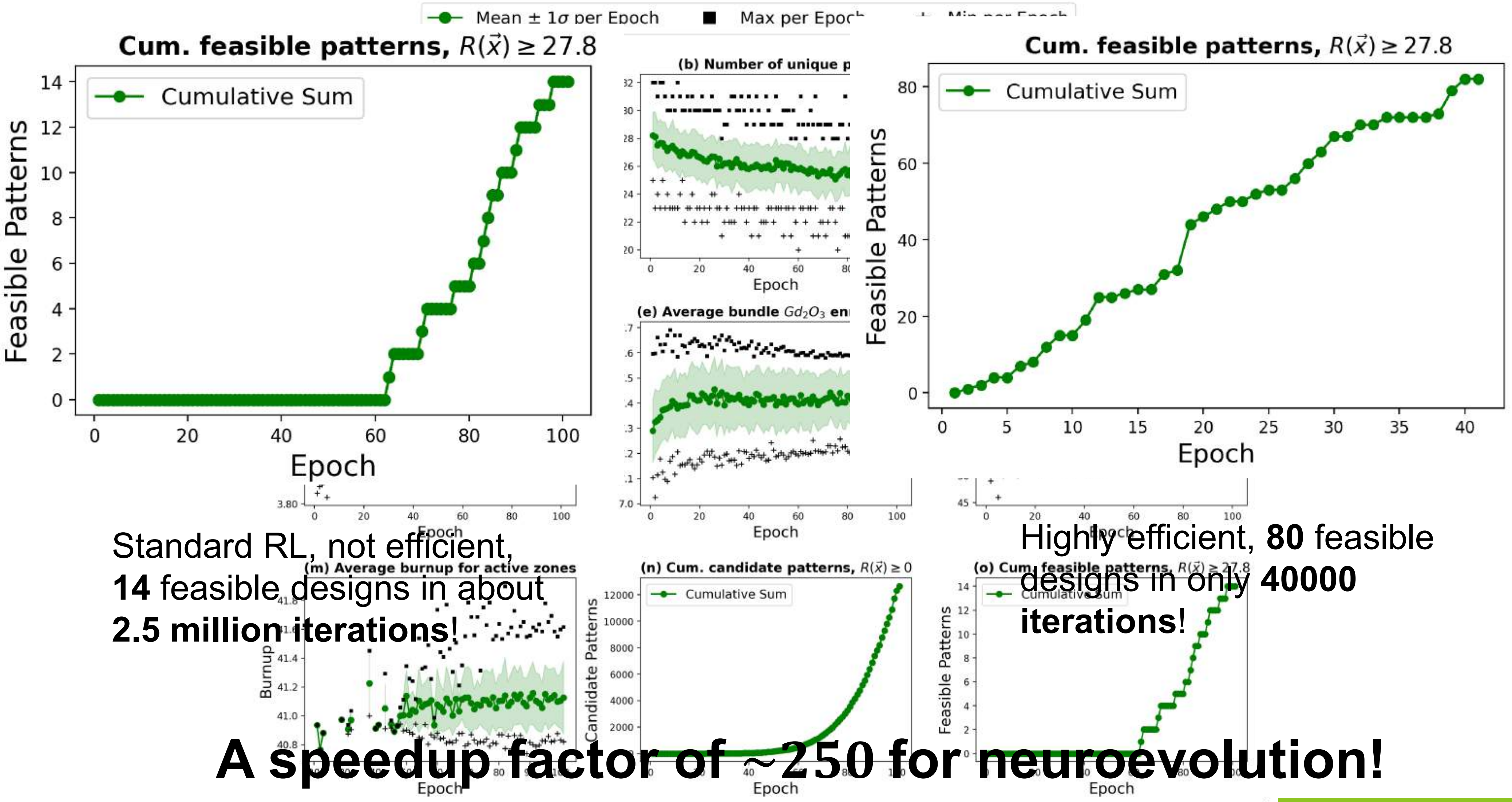
Results



Standard RL, not efficient,
14 feasible designs in about
2.5 million iterations!

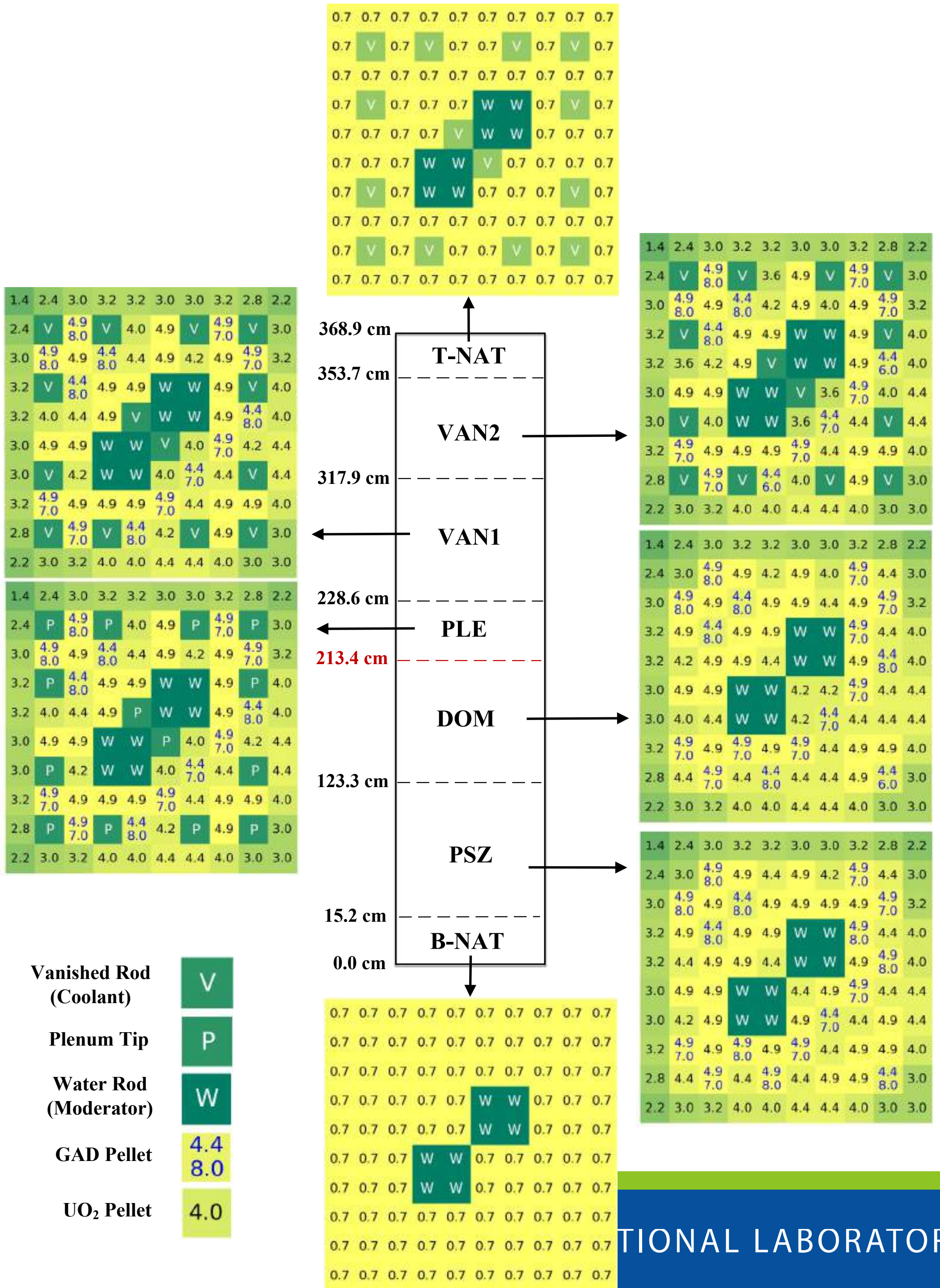
Highly efficient, **80** feasible designs in only **40000 iterations**!

A speedup factor of ~250 for neuroevolution!

Radaideh, M. I., Forget, B., Shirvan, K. (2021). Large-scale design optimisation of boiling water reactor bundles with neuroevolution. *Annals of Nuclear Energy*, *160*, 108355.

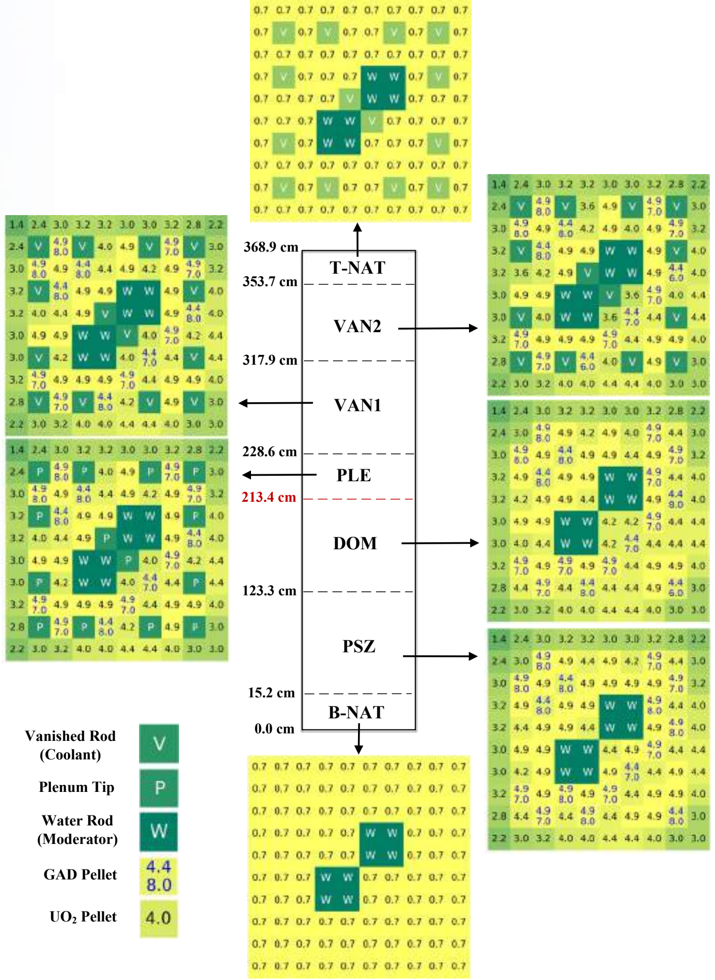
Looking Ahead

- With **NO** human intervention, fully optimized bundle by a **neuroevolution algorithms.**
- Fuel engineers at Exelon are getting **reduced design efforts**.
- The results are **very competitive to the designs used by Exelon/GE**.
- The search can be done in **12-24 hrs using a modest computing power of 32 processors!**
- When scaled to the full core, **expected savings on fuel costs are about 3 million dollars**
  - Still a preliminary guess, core optimization is on the road for future work.



Questions?


TIME 0:08
RINGS 10


368.9 cm
T-NAT
353.7 cm
VAN2
317.9 cm
VAN1
228.6 cm
PLE
213.4 cm
DOM
123.3 cm
PSZ
15.2 cm
B-NAT
0.0 cm
Vanished Rod (Coolant)
V
Plenum Tip
P
Water Rod (Moderator)
W
GAD Pellet
4.4
8.0
UO₂ Pellet
4.0

Robust Data-Driven Sensor Placement

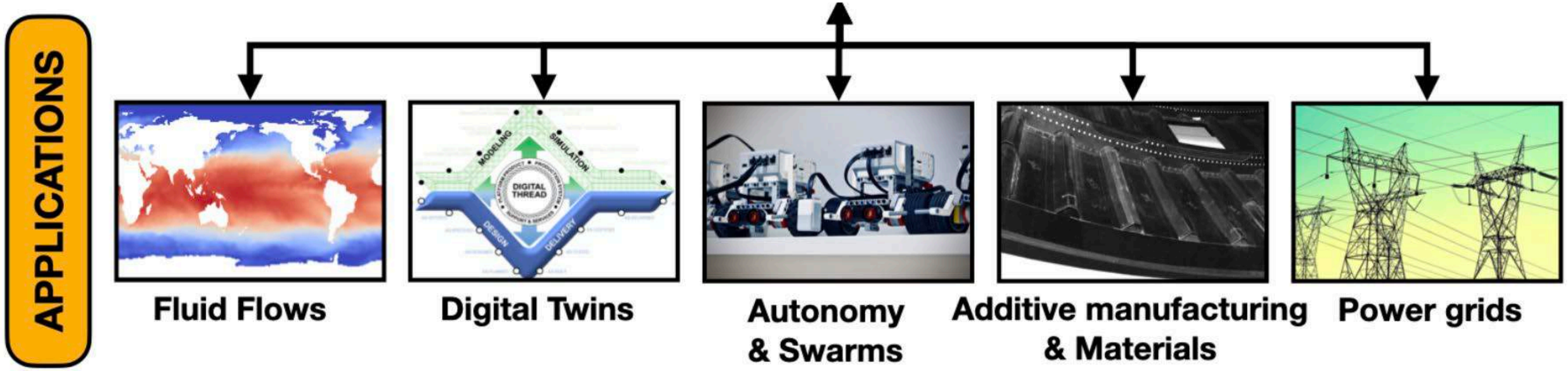
Krithika Manohar
University of Washington

June 8, 2021


Collaborators
Steven L. Brunton, UW
J. Nathan Kutz, UW

Scalable + optimal sensor placement

- Measurements crucial for prediction and control of complex systems
  - Expensive to deploy
  - Spatial constraints on placement
  - Governing models unavailable
- **Our approach**: Robust, data-driven sensor placement
  - Extract low-dimensional structure from data using ML
  - Sparse sensing to determine important locations in state space



kmanohar@uw.edu

Scalable + optimal sensor placement

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  - Extract low-dimensional structure from data using ML
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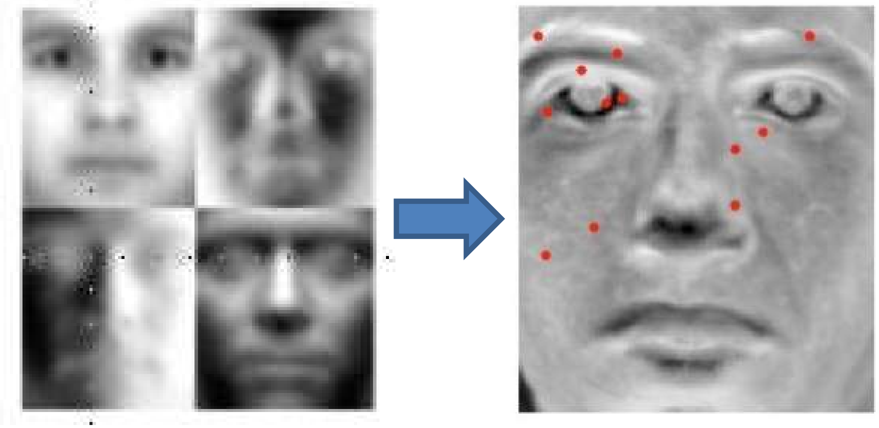
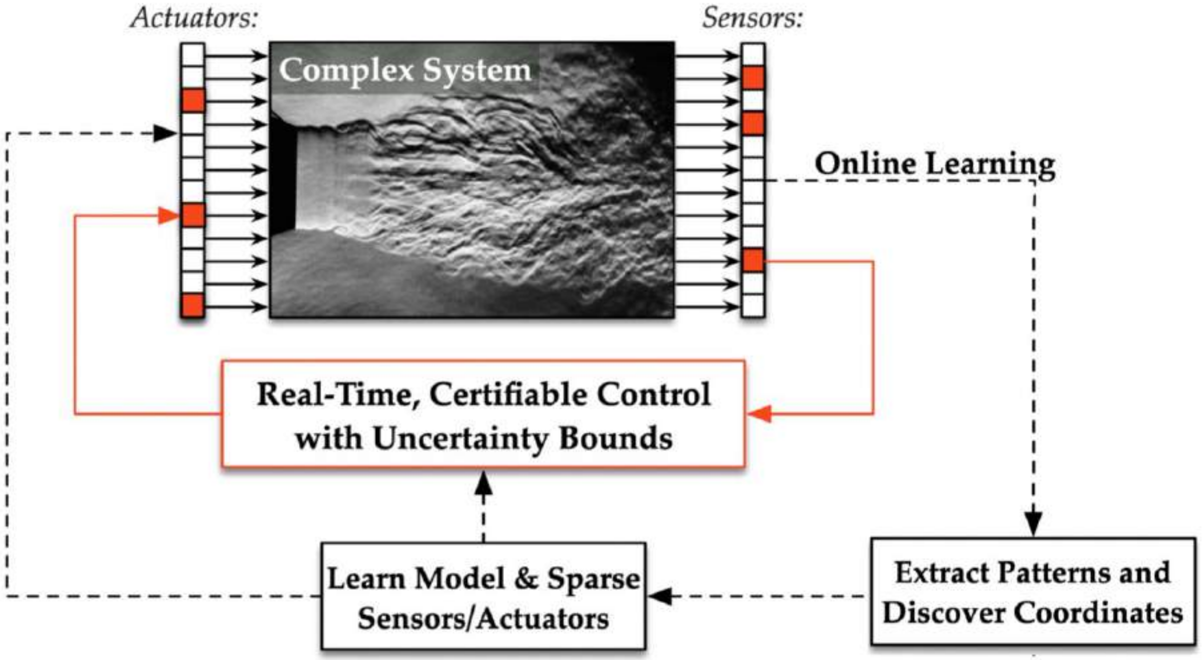
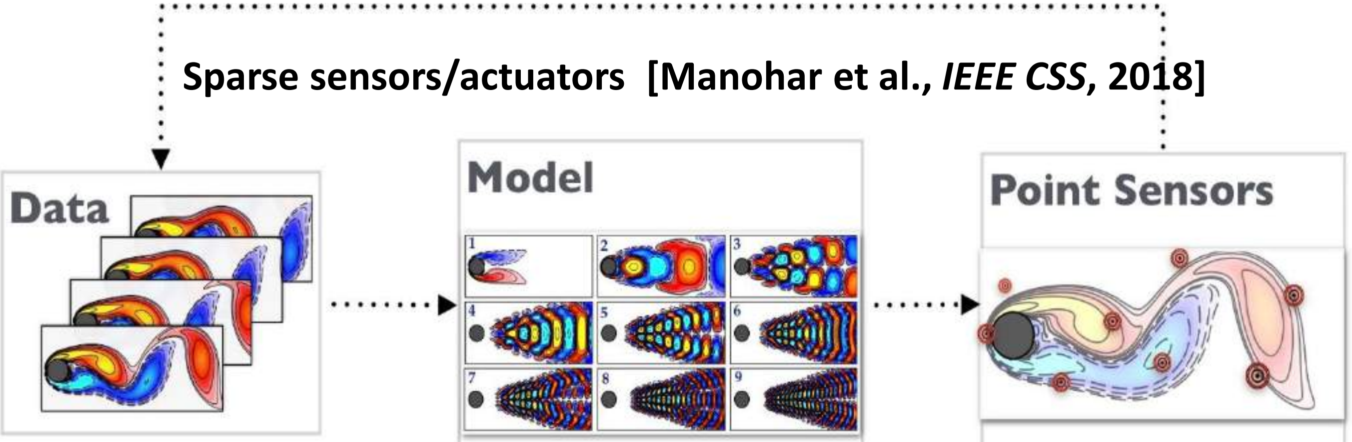
Sensors for classification, [Brunton et al]



Overview

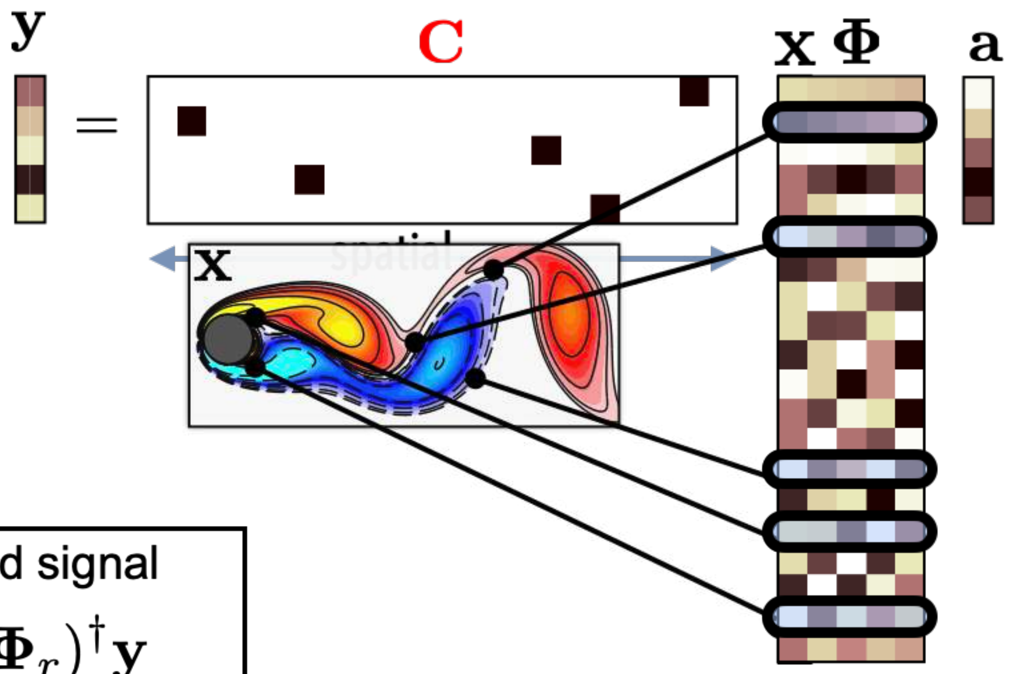


Sparse sensors/actuators [Manohar et al., *IEEE CSS*, 2018]



Sparse sensing for reconstruction

- Reconstruct **x** from measurements **y** in a basis of descriptive features
  - Recover coefficients **a** of **x** in basis (*gappy POD, Everson & Sirovich 1995*)
- Design sensing matrix **C** to minimize error covariance of estimate



$$\mathbf{x} \approx \mathbf{\Phi}_r \mathbf{a}$$

$$\mathbf{y} = \mathbf{C}\mathbf{x} + \boldsymbol{\eta}$$

$$\approx \mathbf{C}\mathbf{\Phi}_r \mathbf{a} + \boldsymbol{\eta}$$

Recovered signal

$$\hat{\mathbf{a}} = (\mathbf{C}\mathbf{\Phi}_r)^\dagger \mathbf{y}$$

$$\hat{\mathbf{x}} = \mathbf{\Phi}_r(\mathbf{C}\mathbf{\Phi}_r)^\dagger \mathbf{y}$$

Sparse sensing for reconstruction

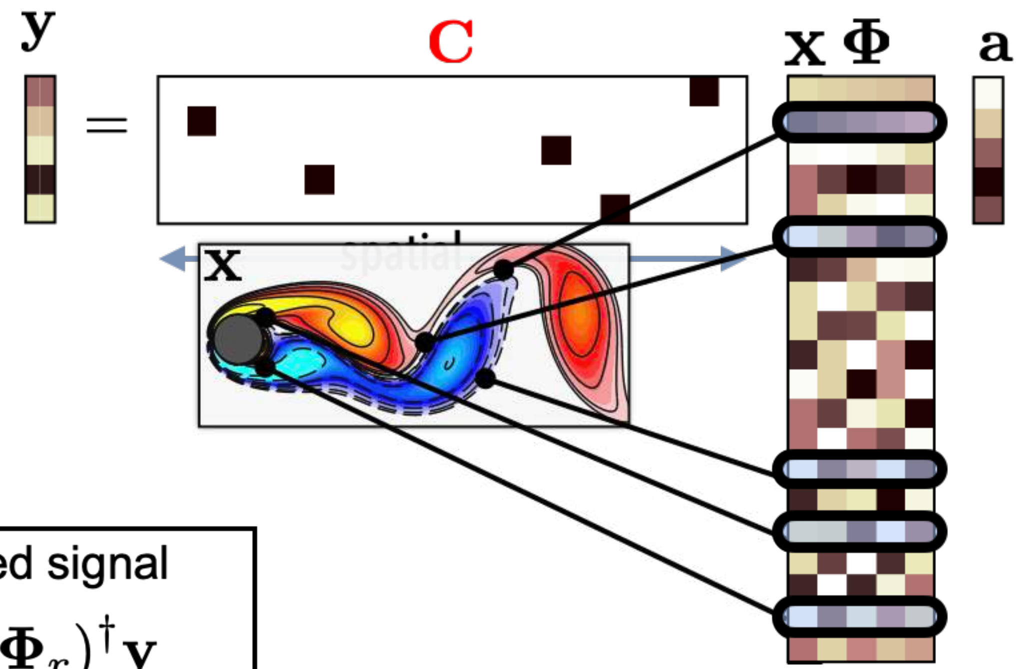
- Reconstruct **x** from measurements **y** in a basis of descriptive features
  - Recover coefficients **a** of **x** in basis (*gappy POD, Everson & Sirovich 1995*)
- Design sensing matrix **C** to minimize error covariance of estimate

$$\mathrm{Var}[\mathbf{a} - \hat{\mathbf{a}}] = \sigma^2[(\mathbf{C}\boldsymbol{\Phi}_r)^T\mathbf{C}\boldsymbol{\Phi}_r]^{-1}$$

$$\max_{\mathbf{C}\in\mathbb{R}^{q\times n}} \det(\mathbf{C}\boldsymbol{\Phi}_r)^T\mathbf{C}\boldsymbol{\Phi}_r$$

$$\text{subject to point sensors } \mathbf{C}$$

Brute-force search is NP-hard, scales combinatorially with *N*



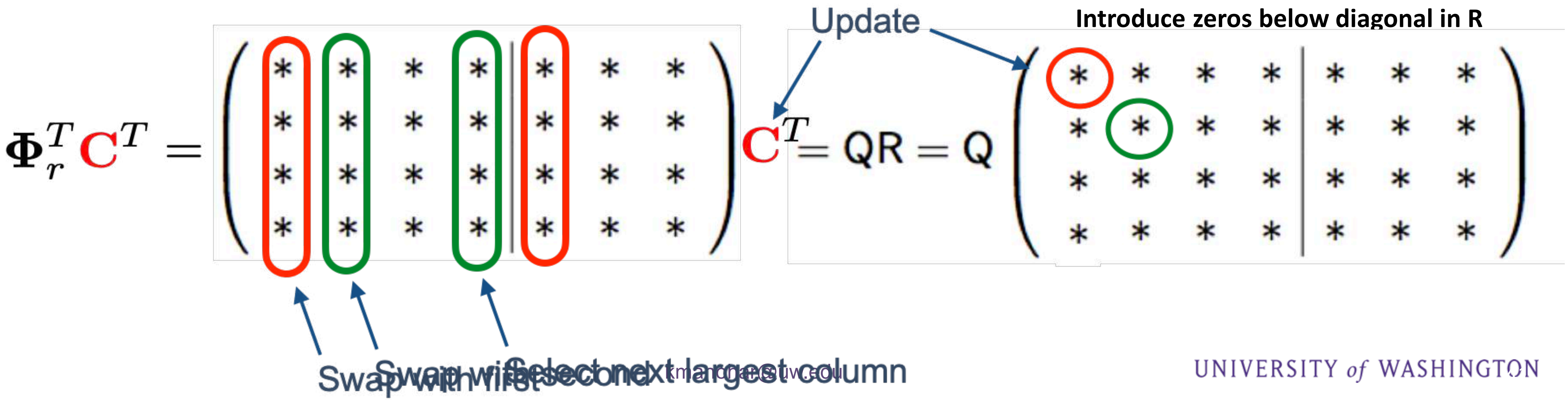
Recovered signal

$$\hat{\mathbf{a}} = (\mathbf{C}\boldsymbol{\Phi}_r)^\dagger\mathbf{y}$$

$$\hat{\mathbf{x}} = \boldsymbol{\Phi}_r(\mathbf{C}\boldsymbol{\Phi}_r)^\dagger\mathbf{y}$$

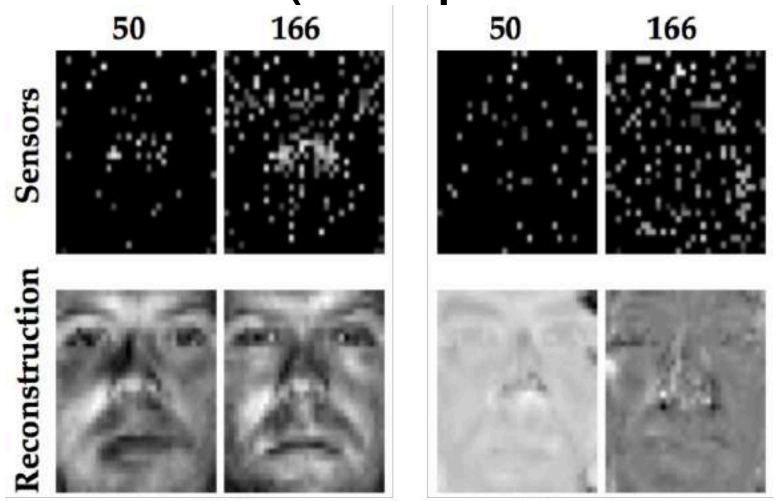
Sparse sensing via QR pivoting

- Factor basis into orthonormal **Q**, upper-triangular **R**, and row permutation **C**
  - Determinant objective = *product of diagonal entries in **R***
  - Use pivoting to introduce diagonally dominant structure
  - *Pivot indices correspond to optimal sensor locations (interpolation points in basis)*
  - Origin: empirical interpolation methods for model reduction **Drmac & Gugercin, SIAM, 2016**

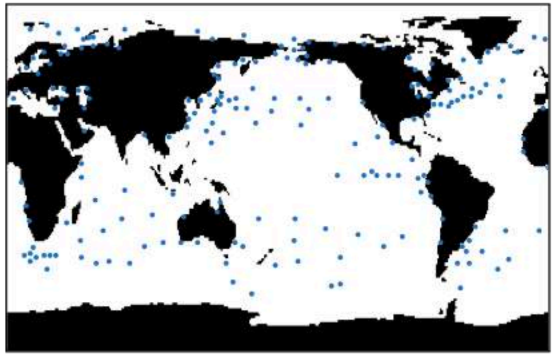


Robust reconstruction

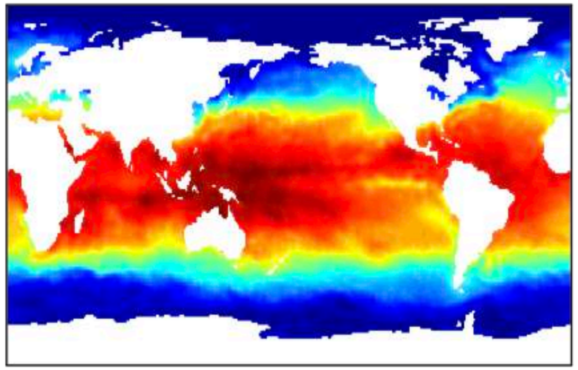
- Reconstruction with minimal number of optimal sensors (compared to random)



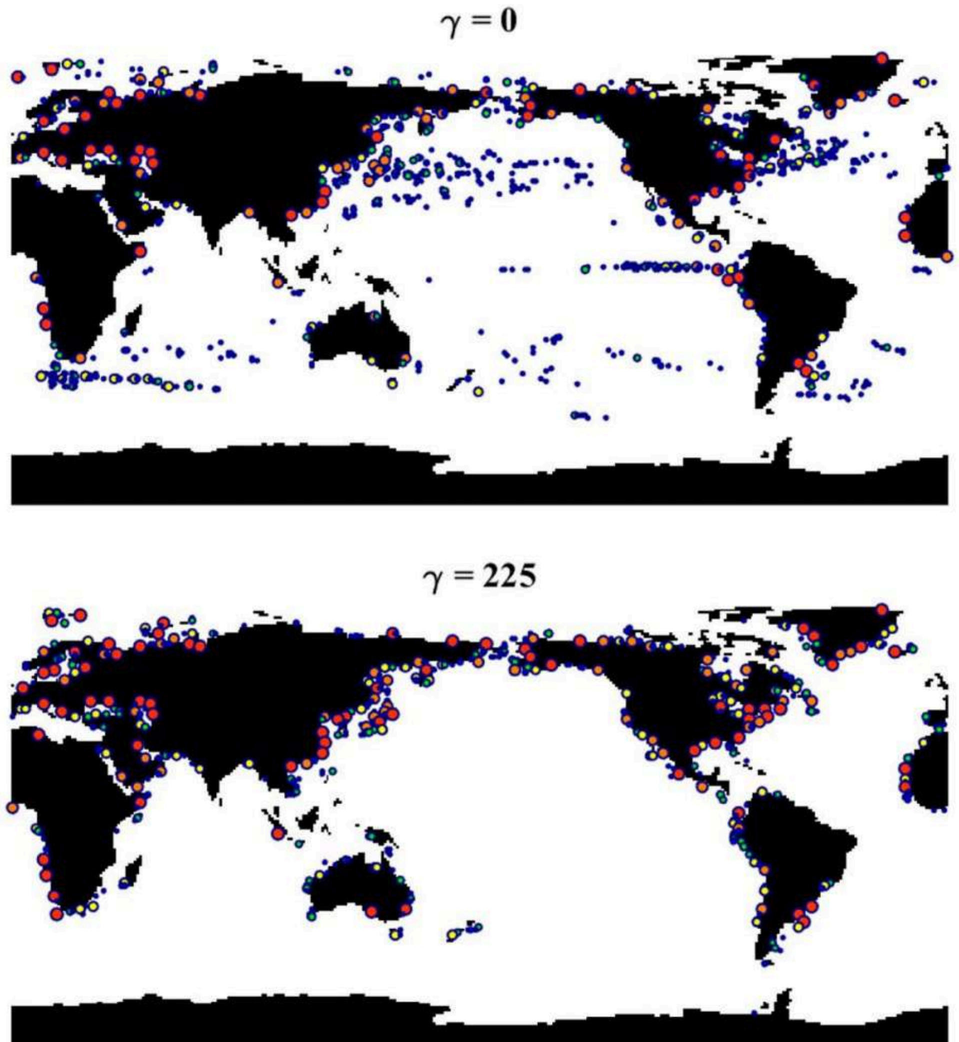
QR Random



200 out of 44219 points



With & Without spatial constraints
[Clark, Askham, Brunton & Kutz 2019]



kmanohar@uw.edu

Robustness

- Interpretable – each sensor corresponds to a principal component (POD mode)
- Feature basis can be adapted to downstream task
  - POD modes ordered by energy content
  - Robust PCA extracts outliers in data
  - Dynamic mode decomposition into spatial modes and frequencies
  - Balanced POD modes ordered by joint controllability and observability
- Adapt model to changing/failing sensors

POD/PCA

$$\mathbf{X} = \mathbf{\Phi}\mathbf{\Sigma}\mathbf{V}^T$$

Robust PCA

$$\min_{\mathbf{L},\mathbf{S}} \|\mathbf{L}\|_* + \quad \|\mathbf{S}\|_1 \text{ such that } \mathbf{L}+\mathbf{S}=\mathbf{X}$$

DMD

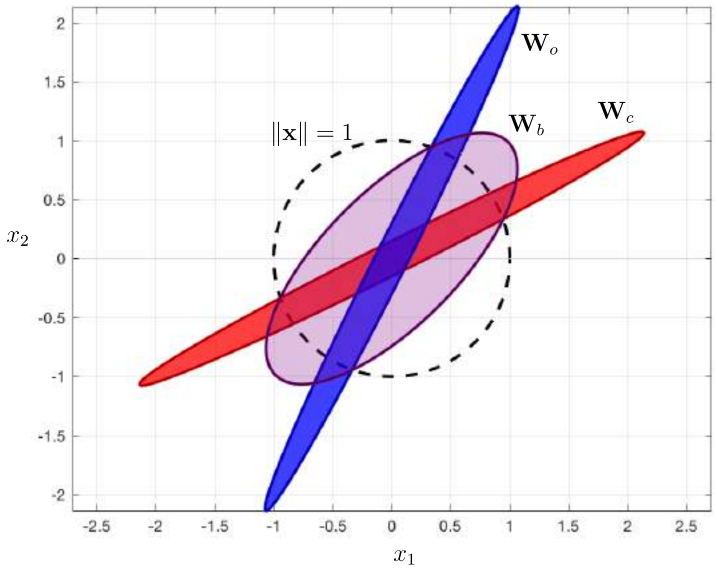
$$\mathbf{x}(t) = \mathbf{\Psi}\,\mathrm{diag}(\exp(\boldsymbol{\omega} t))\mathbf{a}$$

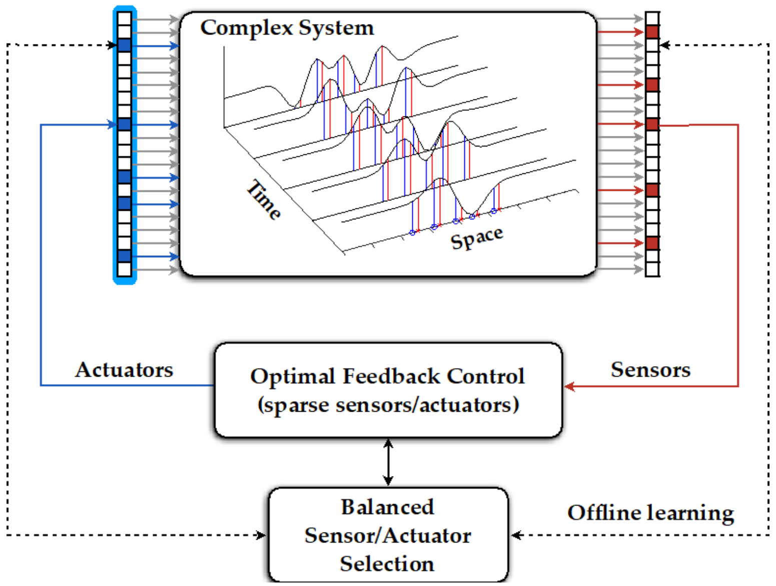
Joint sensor & actuator placement

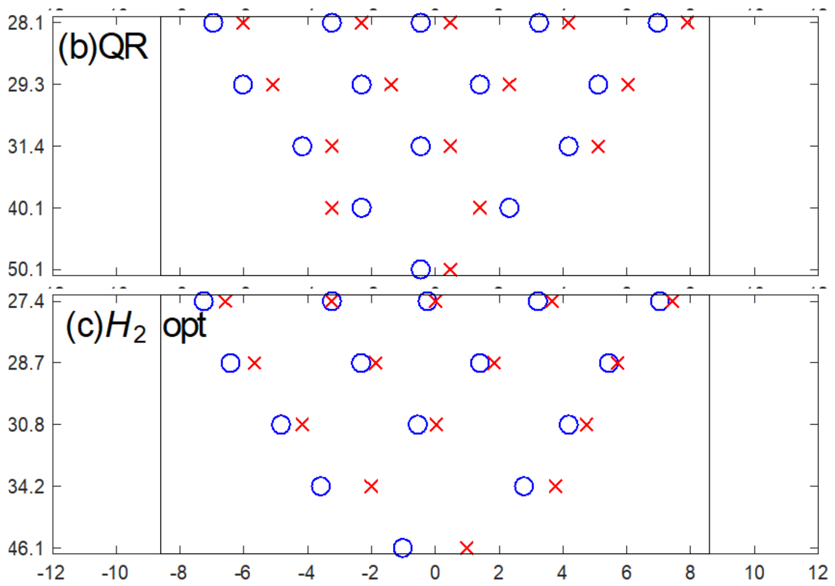
- Optimal sensors and actuations for control
  - Leverage observable/controllable features
  - QR adapted method nearly optimal (bottom right) for linearized Ginzburg–Landau discretized model

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u}$$
$$\mathbf{y} = \mathbf{C}\mathbf{x}$$

Observable and controllable subspaces







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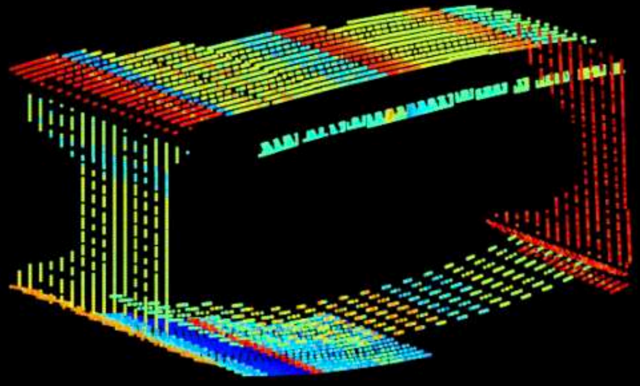
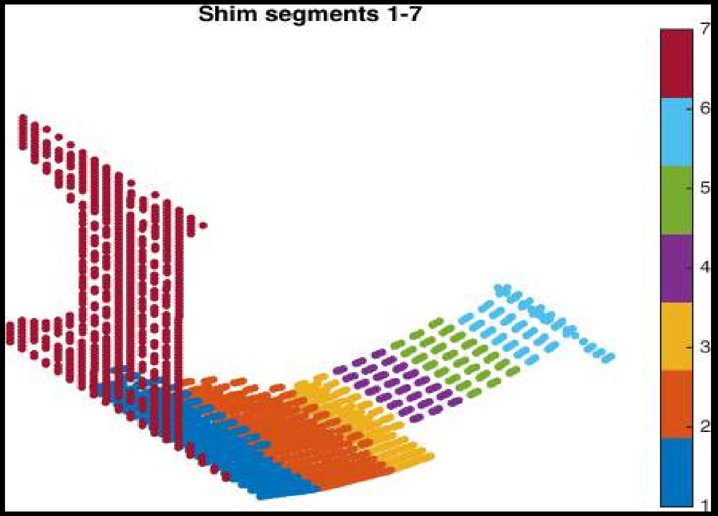
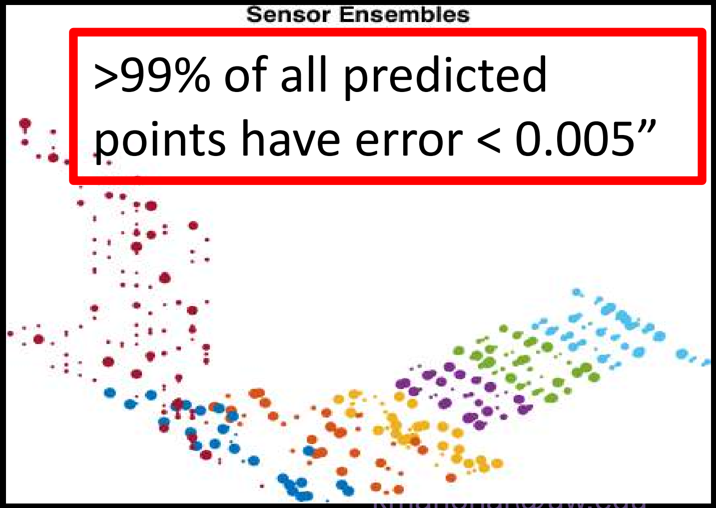
Robust sensors: predictive shimming



Manohar, et al, *J. Manufacturing Systems*, 2018.





References

i. Manohar, Brunton, Kutz & Brunton, "Data-Driven Sparse Sensor Placement for Reconstruction," *IEEE Control Systems*, 38(3):63-86, 2018.

ii. Manohar, Kaiser, Brunton & Kutz, "Optimized sampling of Multiscale Dynamics," *Multiscale Modeling & Simulation,* 17(1):117-136., 2019.

iii. Manohar, Hogan, Buttrick, Banerjee, Kutz & Brunton, "Predicting shim gaps using machine learning and sparse sensing," *J. Manuf. Sys.*, 2018. doi.org/10.1016/j.jmsy.2018.01.011

iv. Manohar, Kutz & Brunton, "Optimal Sensor and Actuator Selection using Balanced Model Reduction", *To appear in IEEE Transactions on Automatic Control,* 2021.

Craig Rieger, PhD, PE

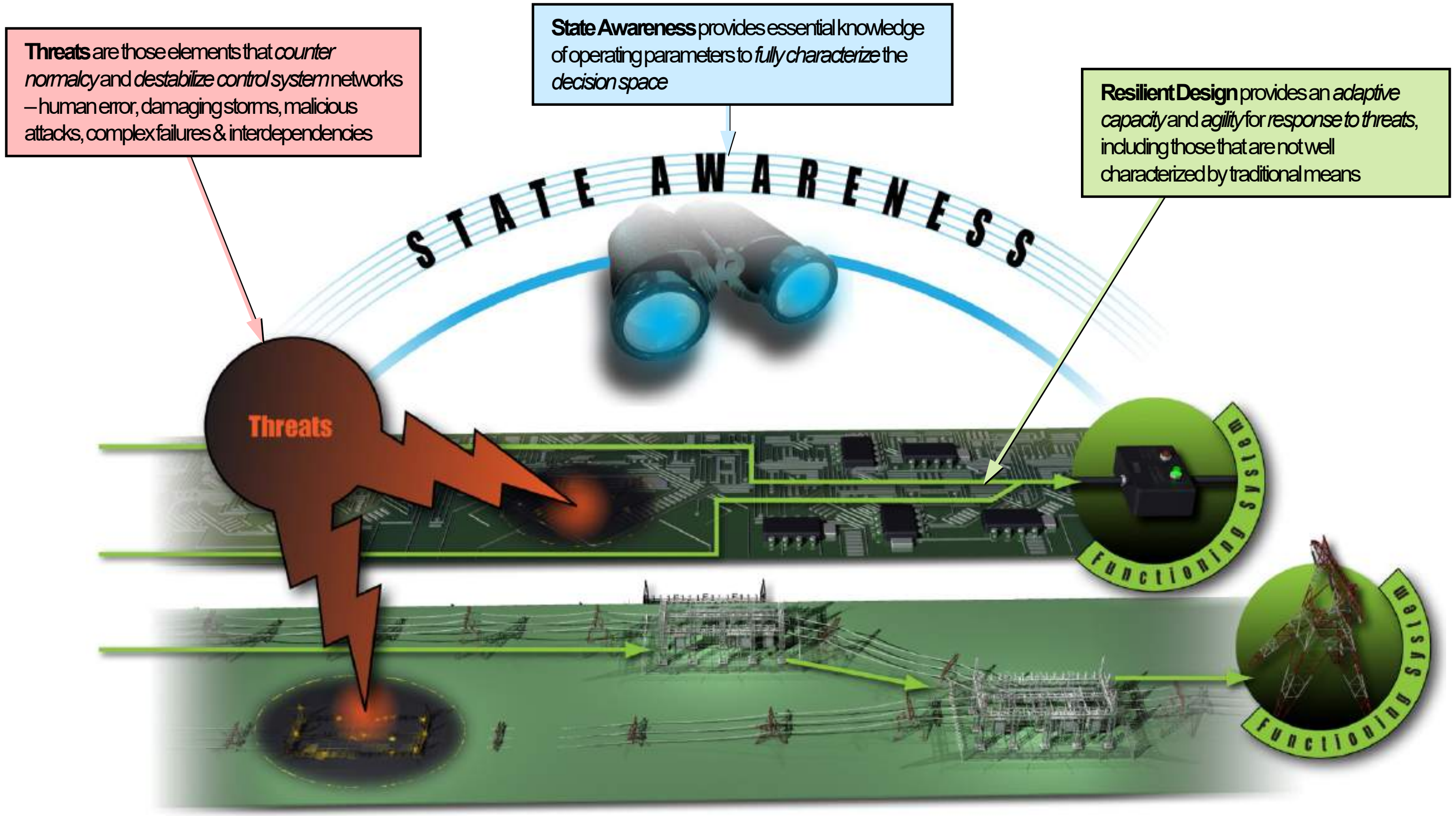
Critical Infrastructure Security and Resilience

Cyber-Physical State Awareness, Automated Response and Confirmed Resilience

Machine Learning & Artificial Intelligence Symposium 5.0

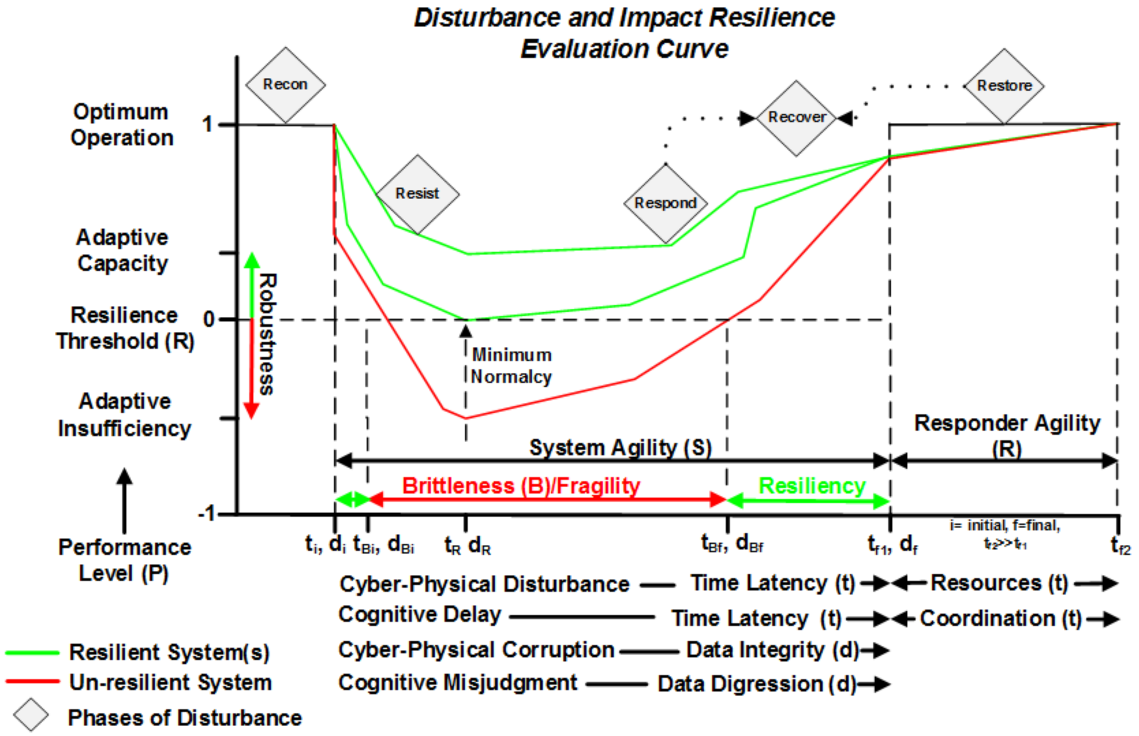
June 8, 2021

Next Generation Control Systems: From Reliable to Resilient



"Resilience" is the capacity of a control system to maintain state awareness and an accepted level of operational normalcy in response to disturbances, including threats of an unexpected and malicious nature. (2009)

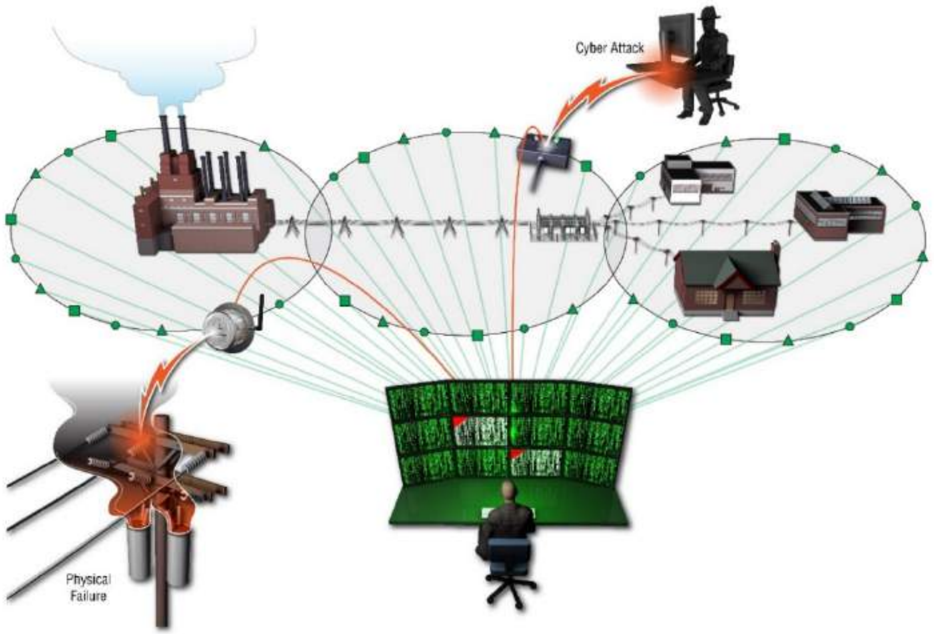
Resilient Control Systems Evaluation



- **Physical Disturbances**
  - Time Latency Affecting Stability
  - Data Integrity Affecting Stability
- **Cyber Disturbances**
  - Time Latency
  - Data Confidentiality, Integrity and Availability
- **Cognitive Disturbances**
  - Time Latency in Response
  - Data Digression from Desired Response
- **Responder**
  - Resources
  - Coordination

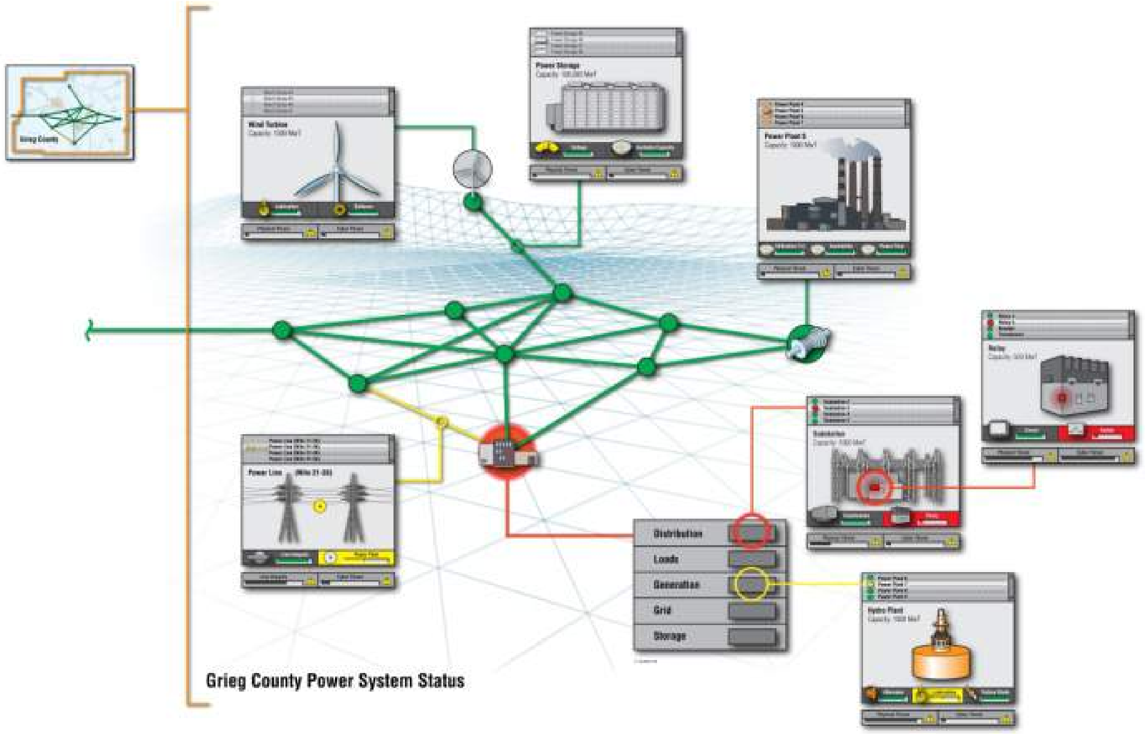
Distributed Infrastructure Cyber-Physical State Awareness

- **Distributed Physical State-awareness**
  - Capability for optimally integrating, monitoring, and controlling the distributed energy systems to prioritize the emergency response to critical infrastructure despite uncertainties.
- **Distributed Cyber State-awareness**
  - Capability for detecting and evaluating cyber threats to allow threat accommodation and reconfiguration of the proposed resilient system against attacks.



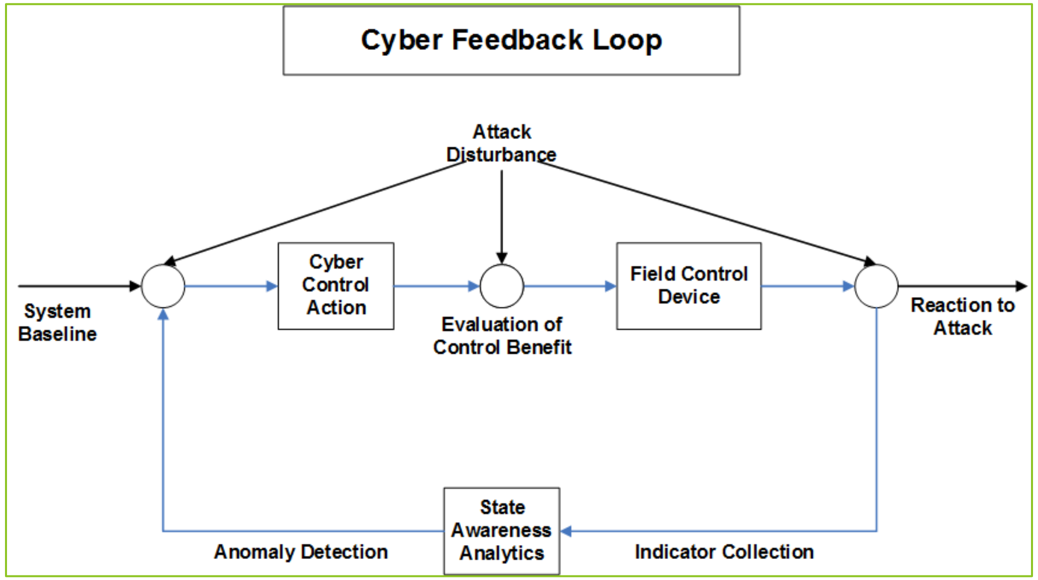
Cyber-Physical Common Operating Visualization

- **Integrated Physical and Cyber State Awareness into a Visualization Engine**
  - The visible aspect of this solution is the display interfaces on devices that present information to humans to make more efficient and effective emergency response



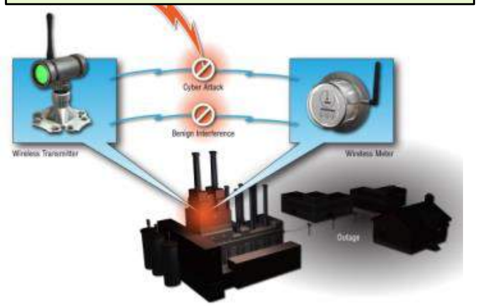
Anomaly Detection and Automated Response& Recovery

- **Cyber-Physical Detection and Analysis of Anomalies**
  - Ingestion of cyber-physical alerts
  - Tradeoff space analysis to validate mitigation benefit and physical impacts that may result
  - Role based actions at the human machine interface
- **Automated Response and Moving Target Defense**
  - Software defined network response actions to redirect or limit traffic for analysis
  - Moving target defenses to deceive actor

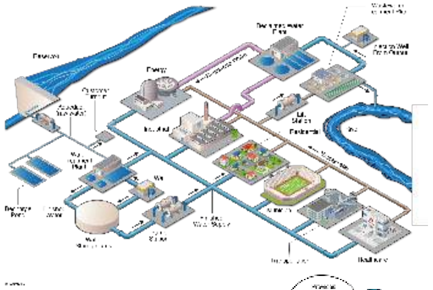


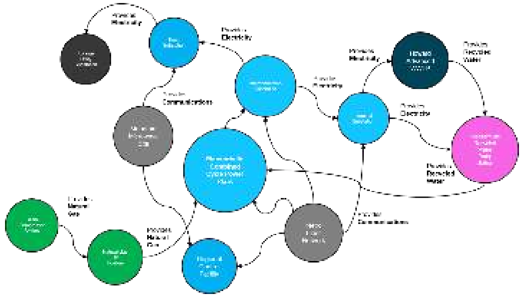
Transformative Research and Deployable Solutions for Inherent Infrastructure Resilience

Intelligent Cyber Detection & Feedback Mechanisms

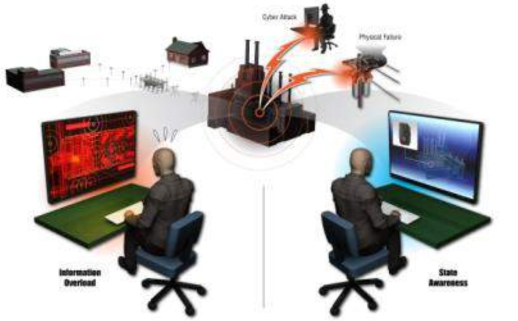


Functional Infrastructure Dependency Modeling for Data Driven Decision Making

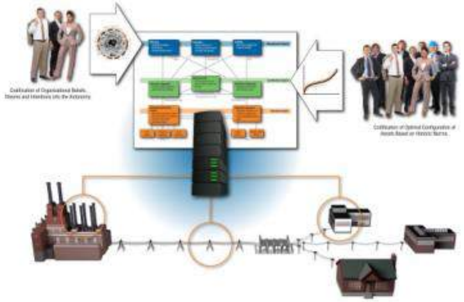




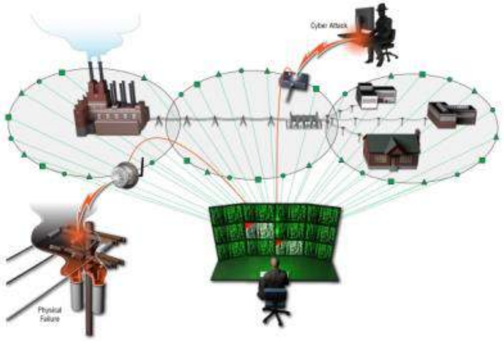
Role-based, Cyber-Physical State and Context Awareness



Adaptive and Agile Resilience Control Architectures



Infrastructure Trustworthiness Assessment & Proactive Control



Annual Symposium

http://www.resilienceweek.com

Join us for the Resilience Week symposium to discuss how private and public partners can work together to ensure a secure and reliable flow of energy across the nation.

- **Topical/Track Areas**
  - Cognitive Systems
  - Communications Systems
  - Control Systems
  - Cyber Systems
  - Critical Infrastructure
  - Communities
  - Industry
- **Participants**
  - DOD/DOE National Labs
  - Cyber-Control-Energy Industries
  - Universities

IEEE Celebrating 125 Years of Engineering the Future

Idaho National Laboratory

Human Factors and Ergonomics Society

Plenaries for 2020

- Jamey Sample, VP CSO (Xcel Energy)
- Kimberly Denbow, Managing Director, Security & Operations (American Gas Association)
- Laura Schepis, Sr Dir, National Security (Edison Electric Institute)
- David Solan, Deputy Assistant Secretary for Renewable Power (EERE)
- Michael Pesin, Deputy Assistant Secretary for Advanced Grid Research and Development (OE)
- Qinghua Li, Associate Professor, Department of Computer Science and Computer Engineering (University of Arkansas)
- Mikhail Falkovich, Director, Information Security (Consolidated Edison Company of New York, Inc.)
- Niyo Little Thunder Pearson, Sr., CISSP, CCSP, Supervisor, Cybersecurity/Cyber Operations (ONE Gas)
- Edward Chiu, Cybersecurity Strategist (Chevron Corp.)
- Chick Macal (Argonne National Laboratory)
- Serena Reynolds, National Risk Management Center (NRMC), Cybersecurity and Infrastructure Security Agency (CISA)
- Amanda Toman, Director of 5G Initiatives (Office of the Under Secretary of Defense)
- Maria Dillard, Acting Director of Disaster and Failure Studies (Engineering Laboratory) (National Institute of Standards and Technology)

Idaho National Laboratory

Idaho National Lab ML-AI Trustworthiness Symposium, June 8, 2021

Human-Centered AI: Reliable, Safe & Trustworthy

Ben Shneiderman `@benbendc`

Founding Director (1983-2000), Human-Computer Interaction Lab
Professor, Department of Computer Science

Member, National Academy of Engineering

Photo: BK Adams

UNIVERSITY OF MARYLAND

HCIL

HUMAN COMPUTER INTERACTION LABORATORY

UNIVERSITY OF MARYLAND 1856

Interdisciplinary research community

- Computer Science & Info Studies
- Psych, Socio, Educ, Jour & MITH

`hcil.umd.edu`

`vimeo.com/72440805`

Designing the User Interface

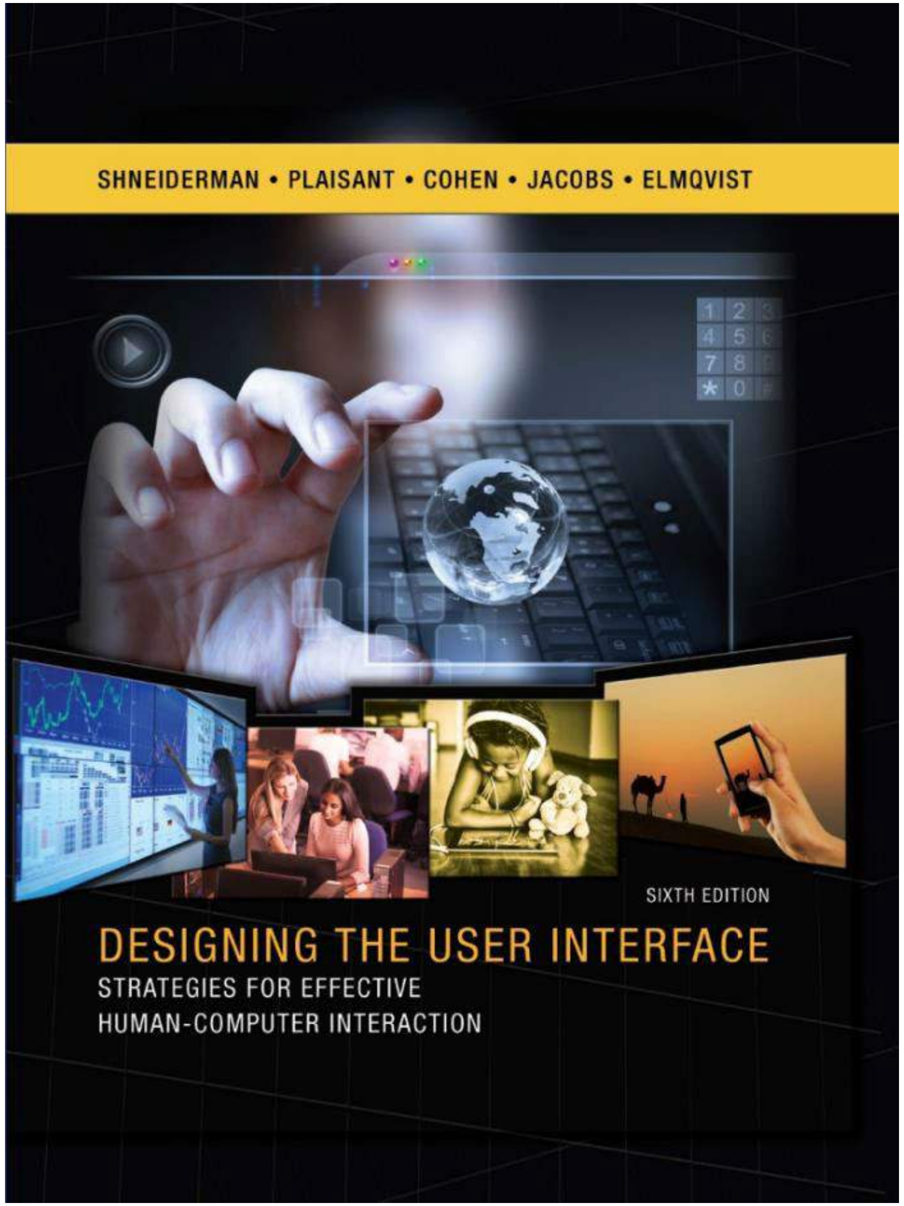
Design Theories

Direct manipulation

Menus, speech, search

Social Media

Information Visualization



www.cs.umd.edu/hcil/DTUI6

Sixth Edition: 2016

Web links

> The **University of Maryland, College Park** (often referred to as the **University of Maryland**, **Maryland**, **UM**, **UMD**, **UMCP**, or **College Park**) is a public research university[10] located in the city of College Park in Prince George's County, Maryland, approximately 4 miles (6.4 km) from the northeast border of Washington, D.C. Founded in 1856, the university is the flagship institution of the University System of Maryland. With a fall 2010 enrollment of more than 37,000 students, over 100 undergraduate majors, and 120 graduate programs,

Tiny touchscreen keyboards

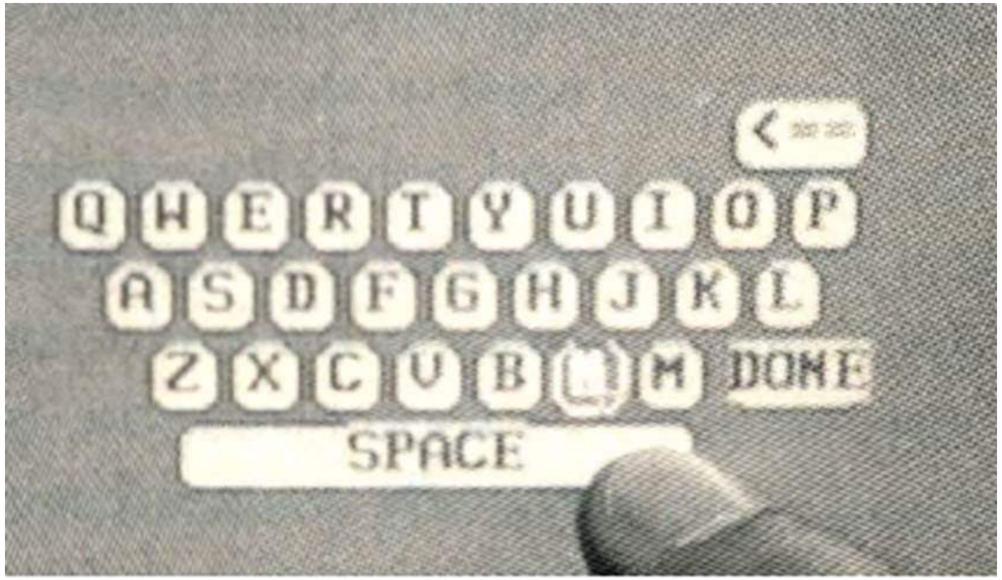
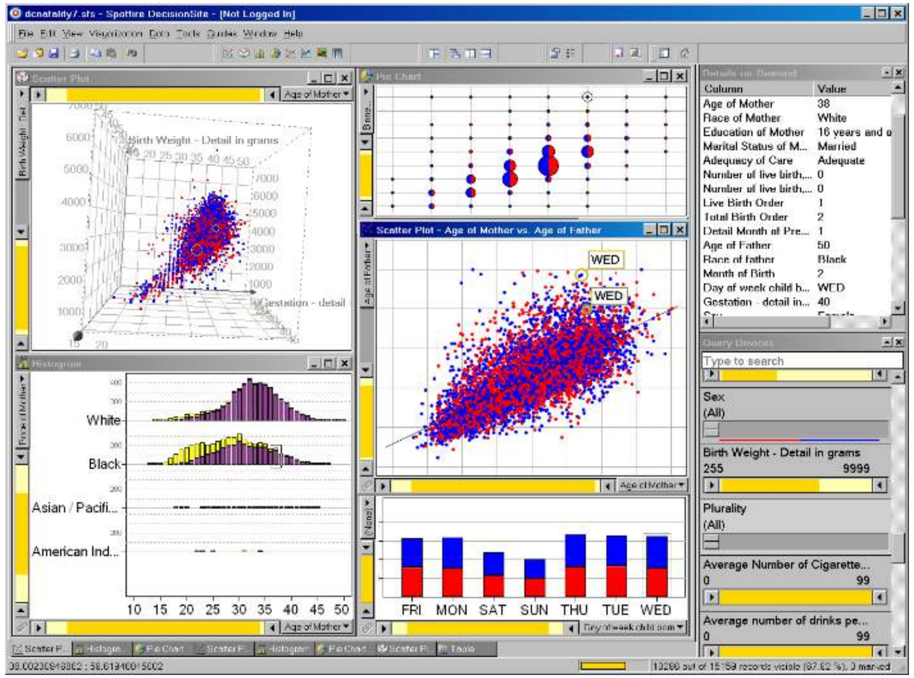
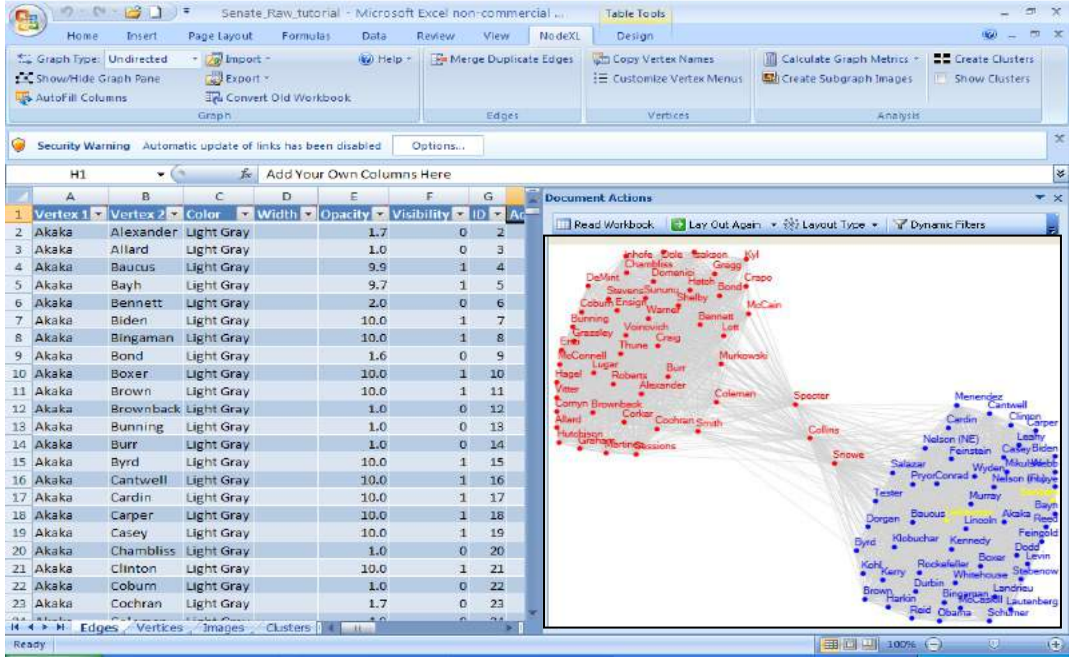


Photo tagging

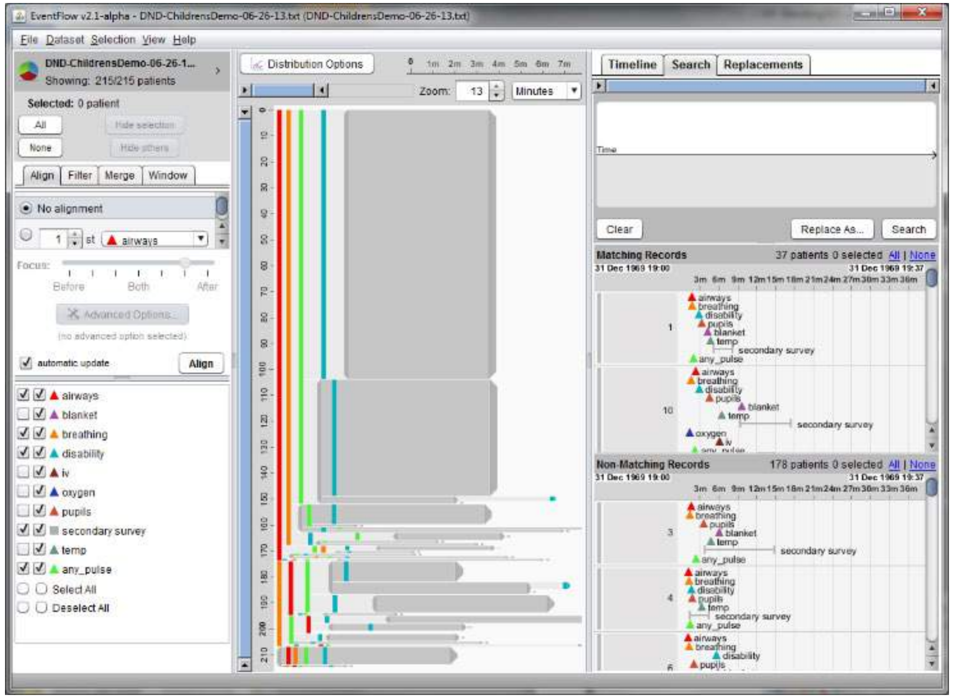


Spotfire

Treemaps
FinViz



NodeXL



EventFlow

What is Human-Centered AI?

What is Human-Centered AI?

Amplify, Augment, Empower & Enhance People

Human-Centered AI

Human Values
Rights, Justice & Dignity

Human-Centered AI

Human Values
Rights, Justice & Dignity

Individual Goals
Self-efficacy, Creativity, Responsibility & Social Connections

Human-Centered AI

Human Values

Rights, Justice & Dignity

Individual Goals

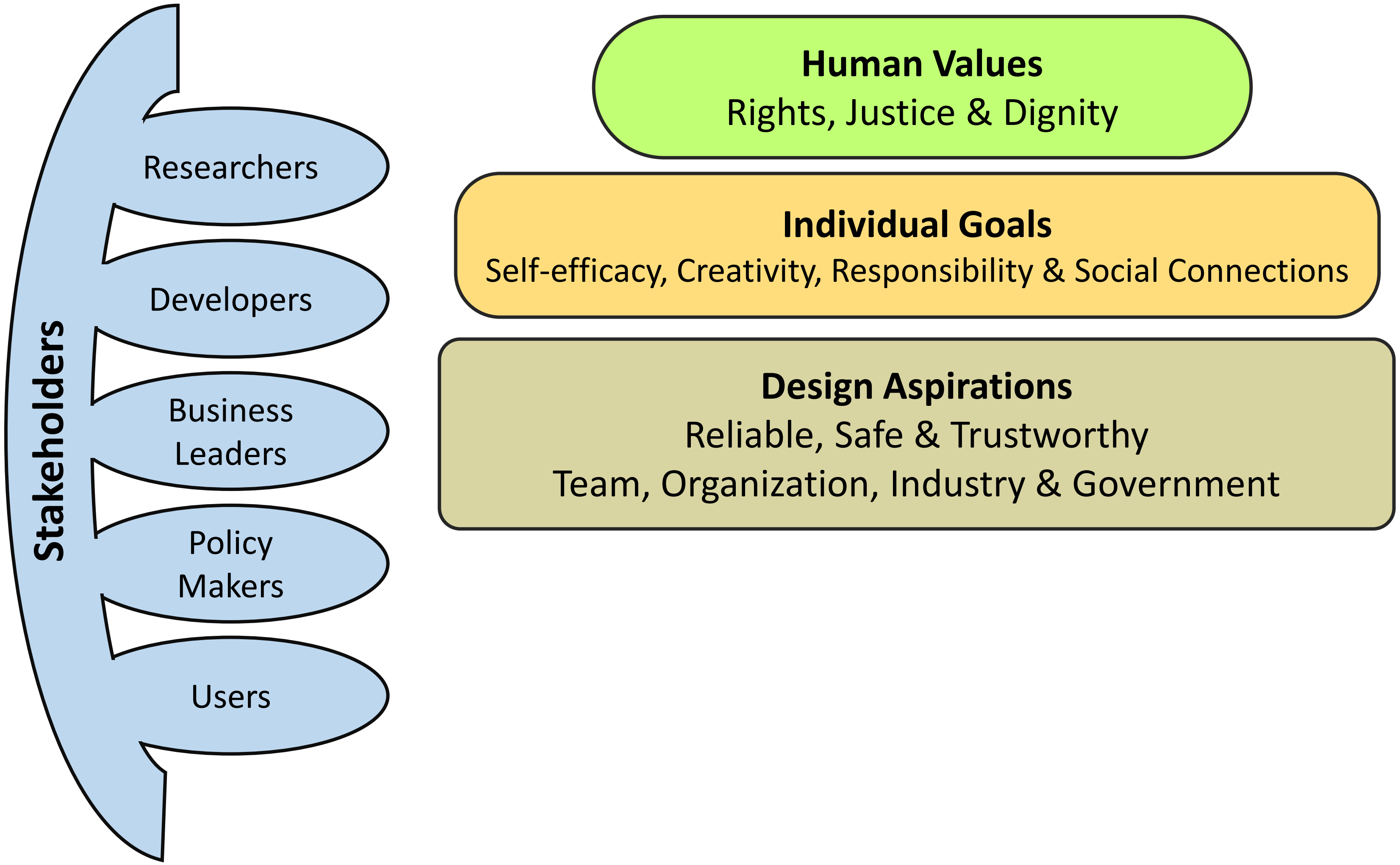
Self-efficacy, Creativity, Responsibility & Social Connections

Design Aspirations

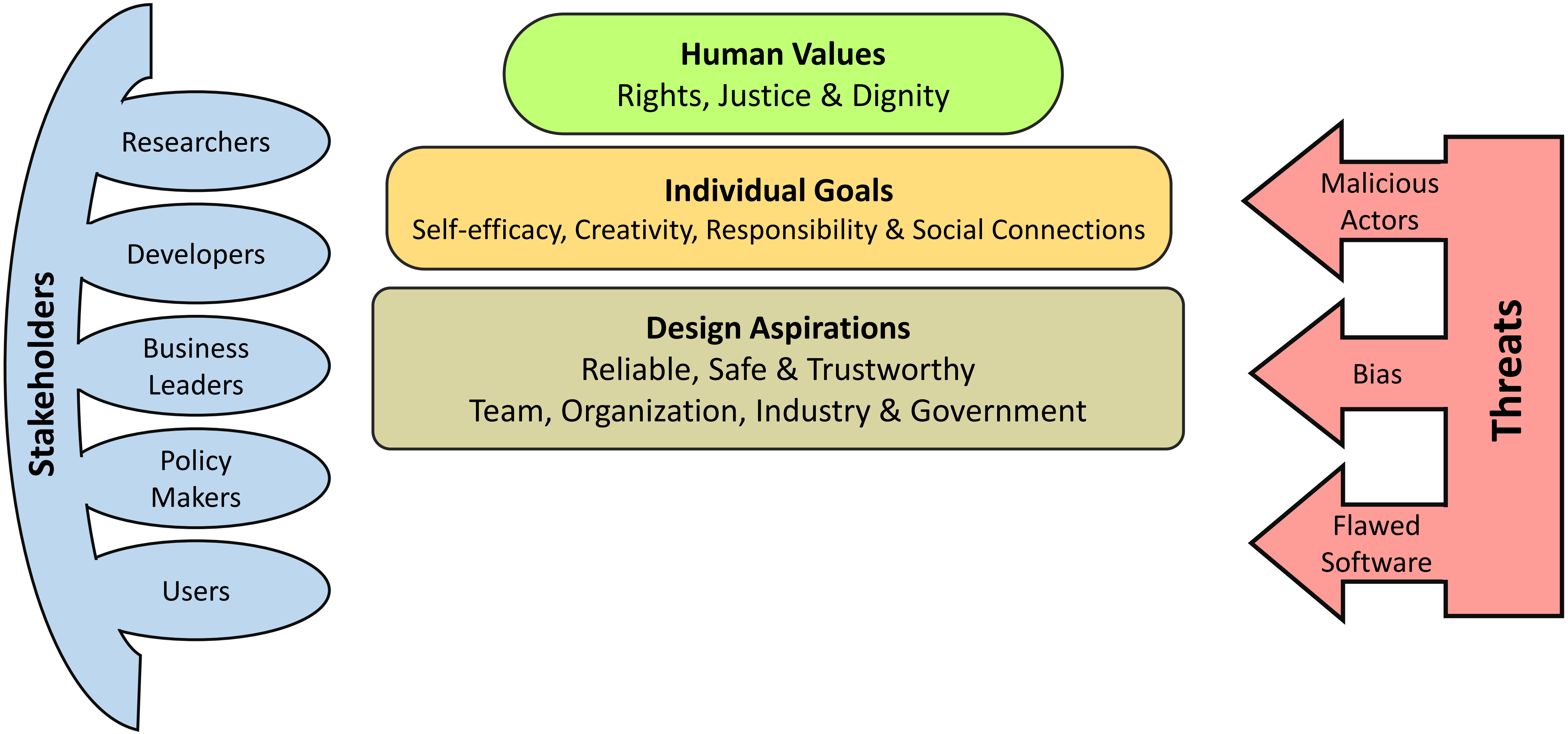
Reliable, Safe & Trustworthy

Team, Organization, Industry & Government

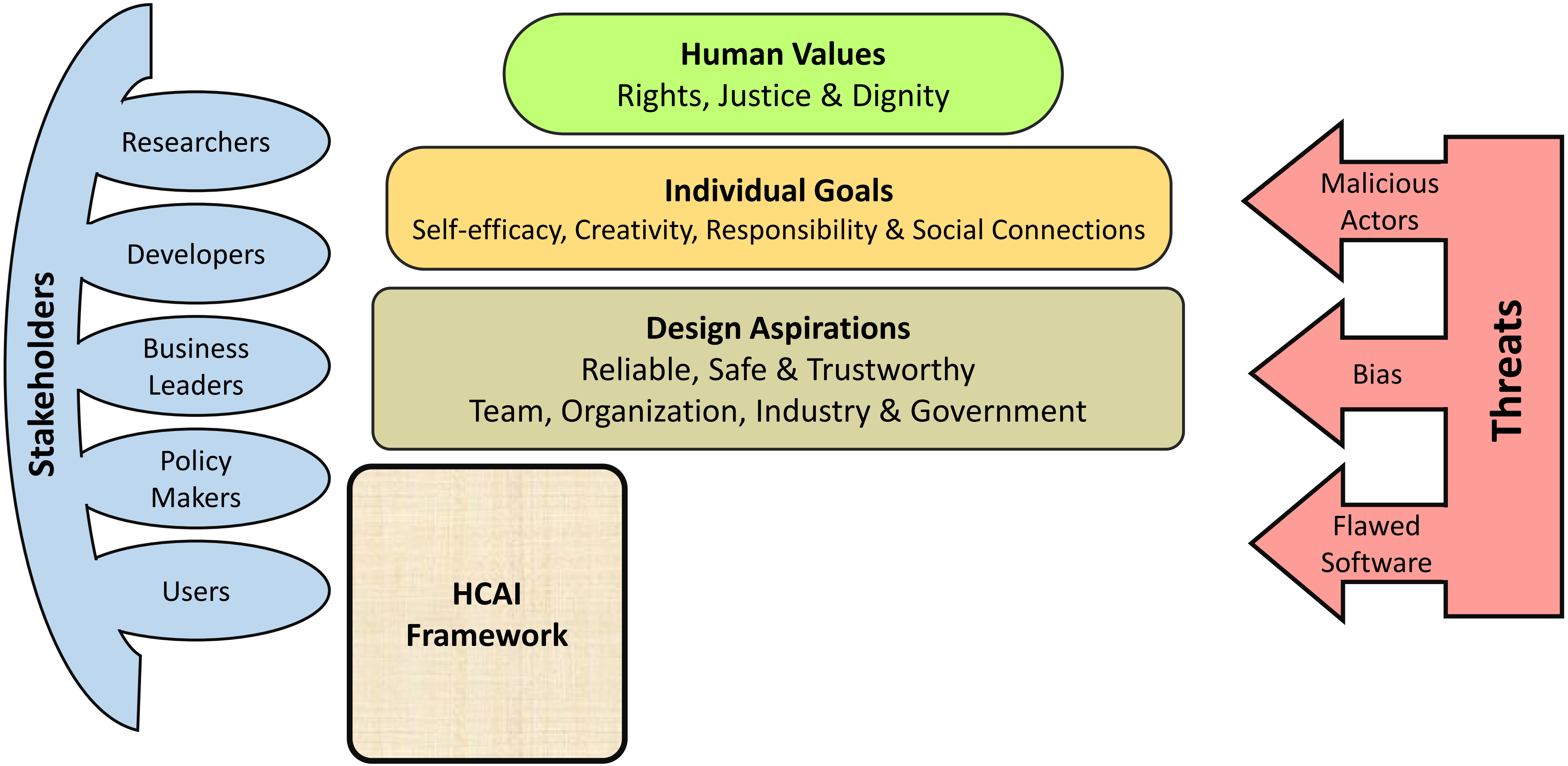
Human-Centered AI



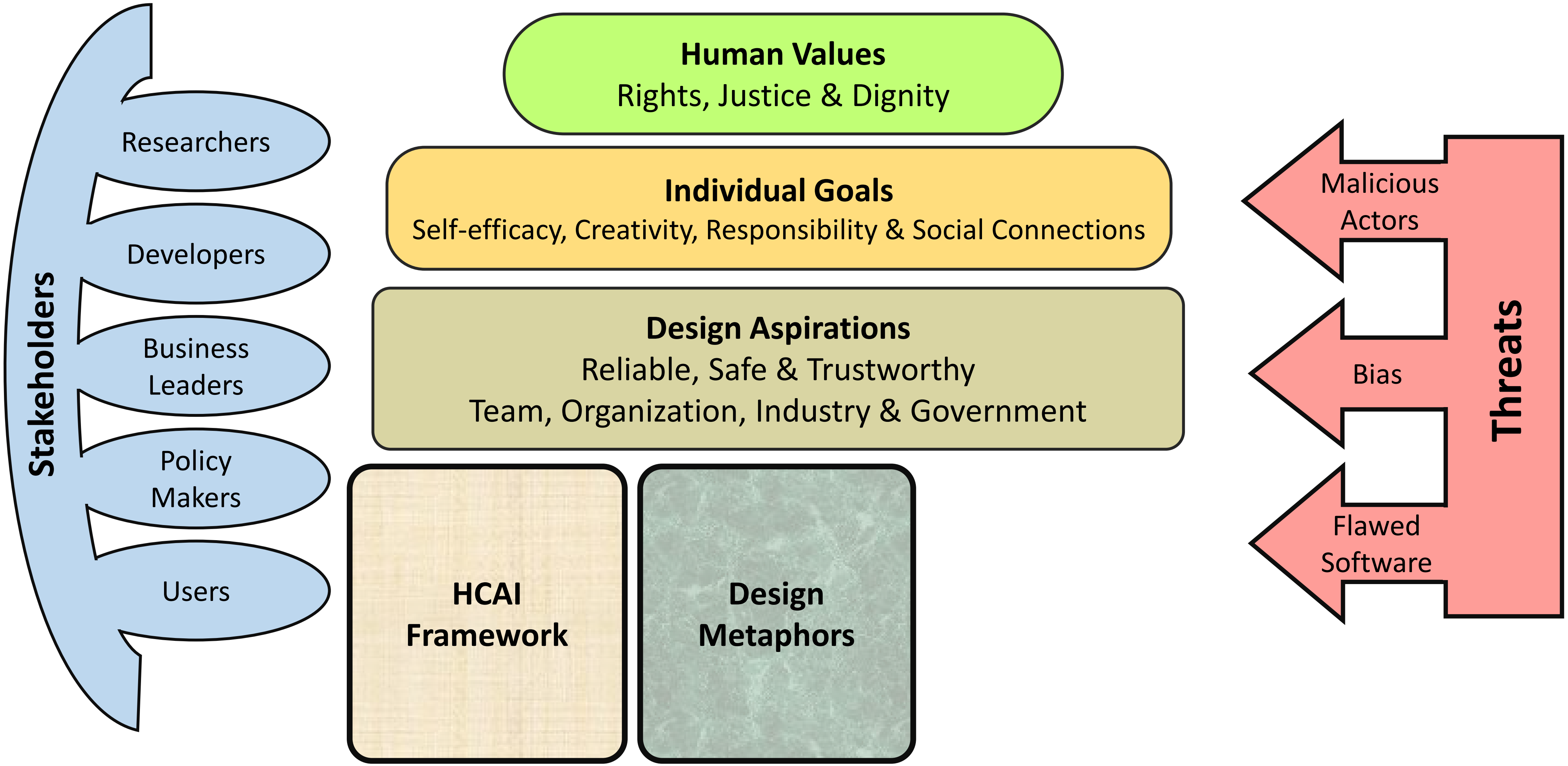
Human-Centered AI



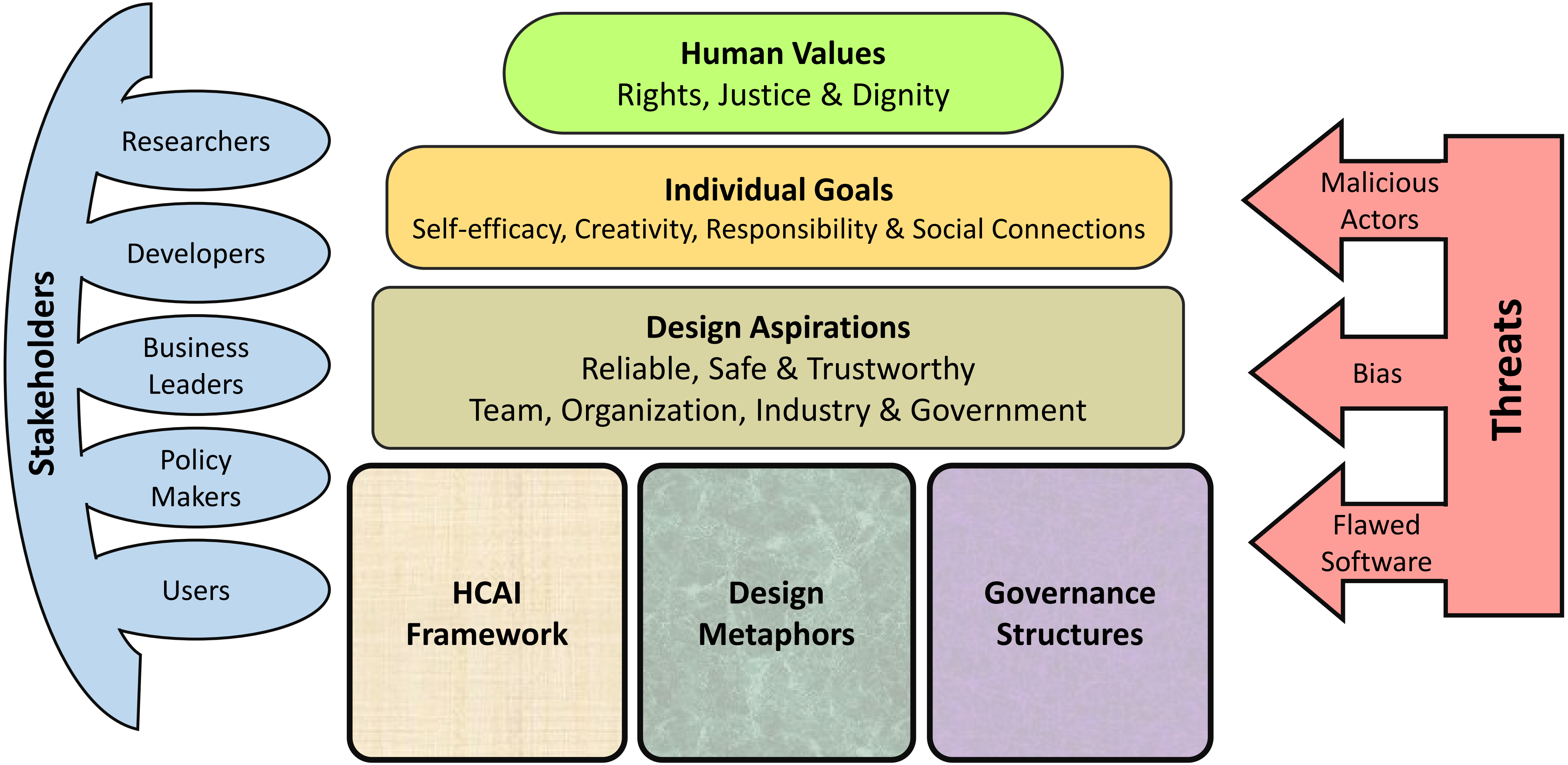
Human-Centered AI



Human-Centered AI



Human-Centered AI

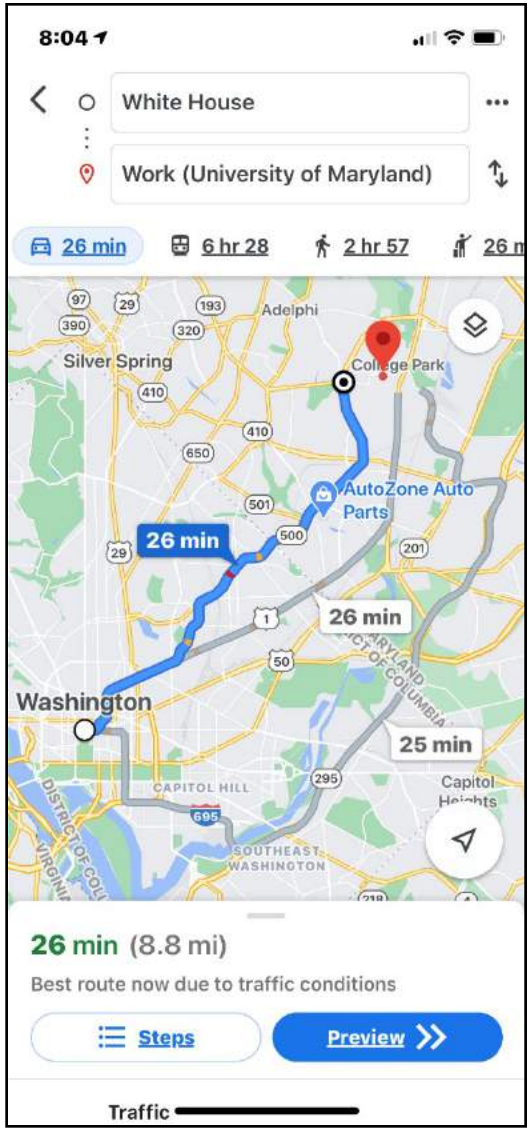


Oxford University Press (Early 2022) `https://hcil.umd.edu/human-centered-ai/`

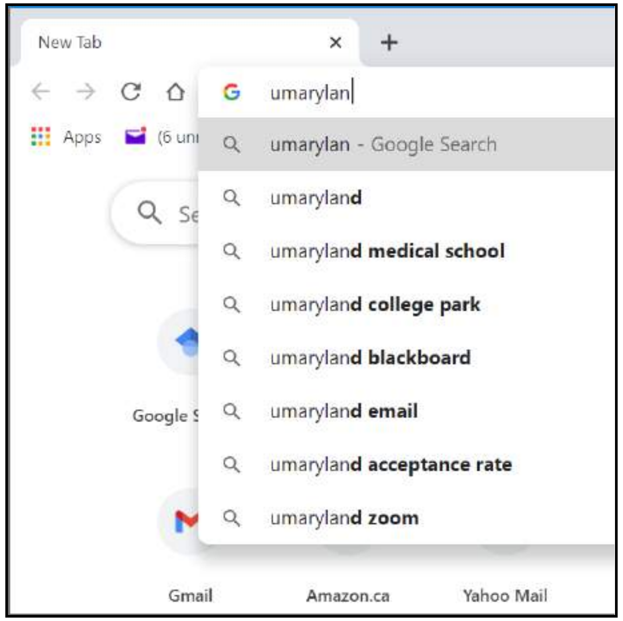
Supertools

Digital Camera Controls

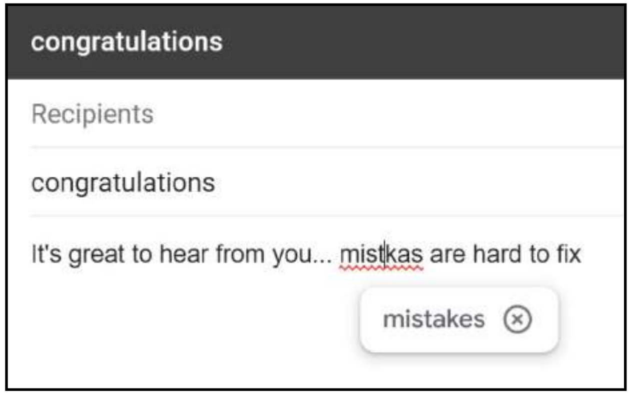
Navigation Choices



Texting Autocompletion



Spelling correction



Active Appliances

Coffee maker, Rice cooker, Blender

Dishwasher, Clothes Washer/Dryer

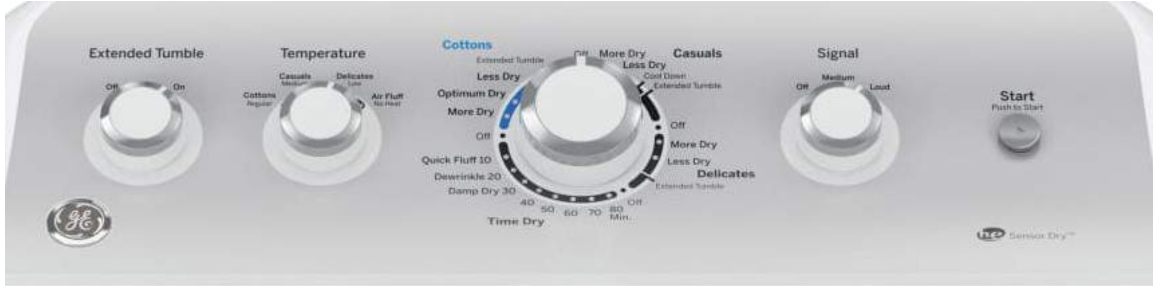
Cuisinart Grind & Brew Coffee Maker

Panasonic Rice Cooker

Nutri Ninja Blender

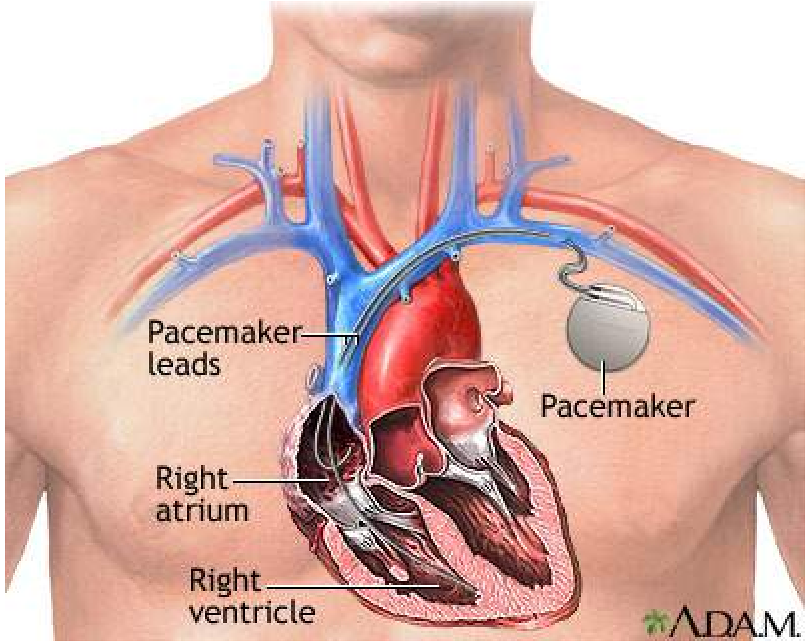
Miele Dishwasher

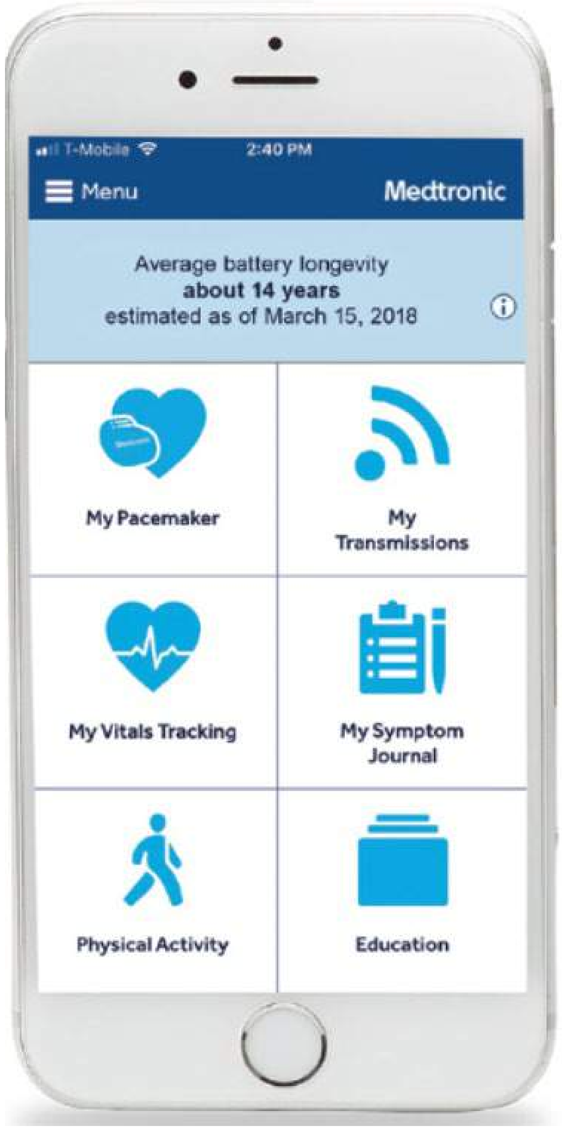
General Electric Washer



General Electric Dryer

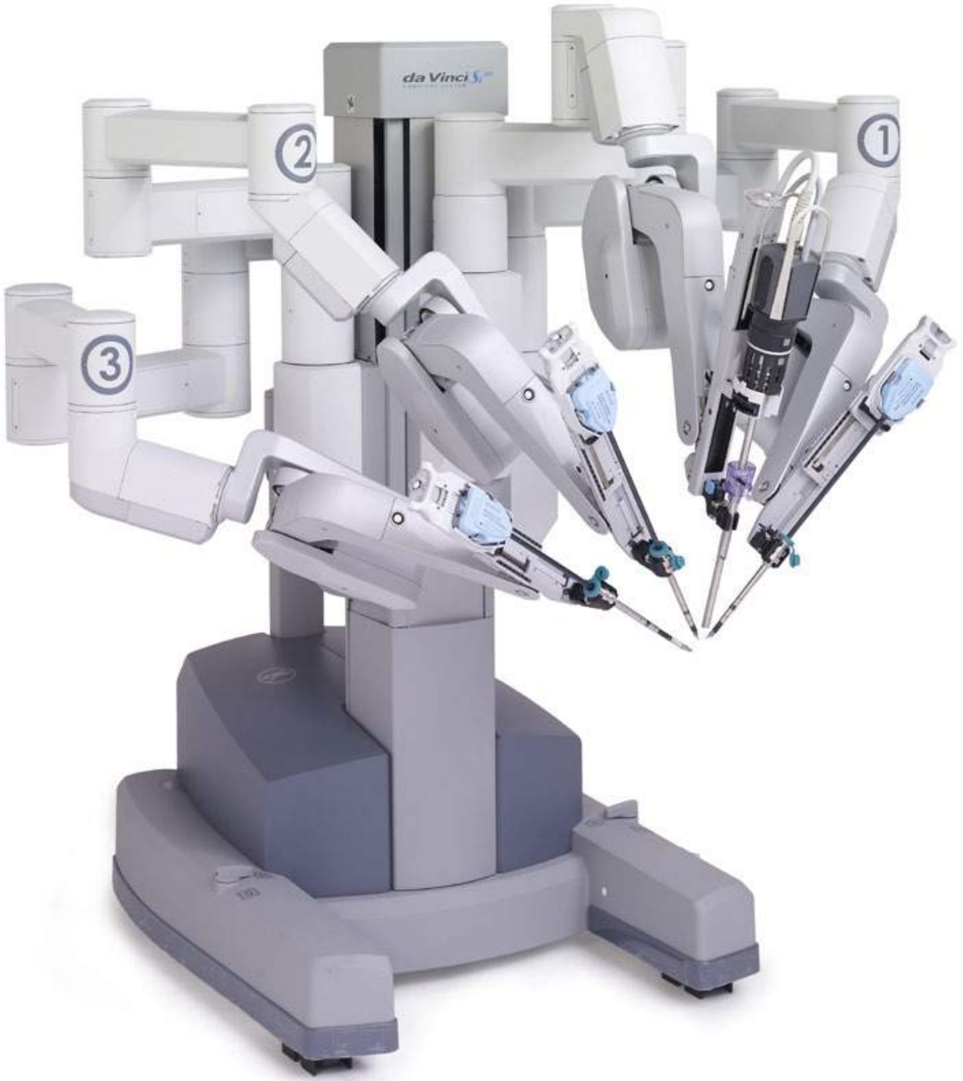
Implanted Cardiac Pacemakers





NASA Mars Rovers are Tele-Operated

Da Vinci Tele-Operated Surgery



"Robots don't perform surgery. Your surgeon performs surgery with da Vinci by using instruments that he or she guides via a console."

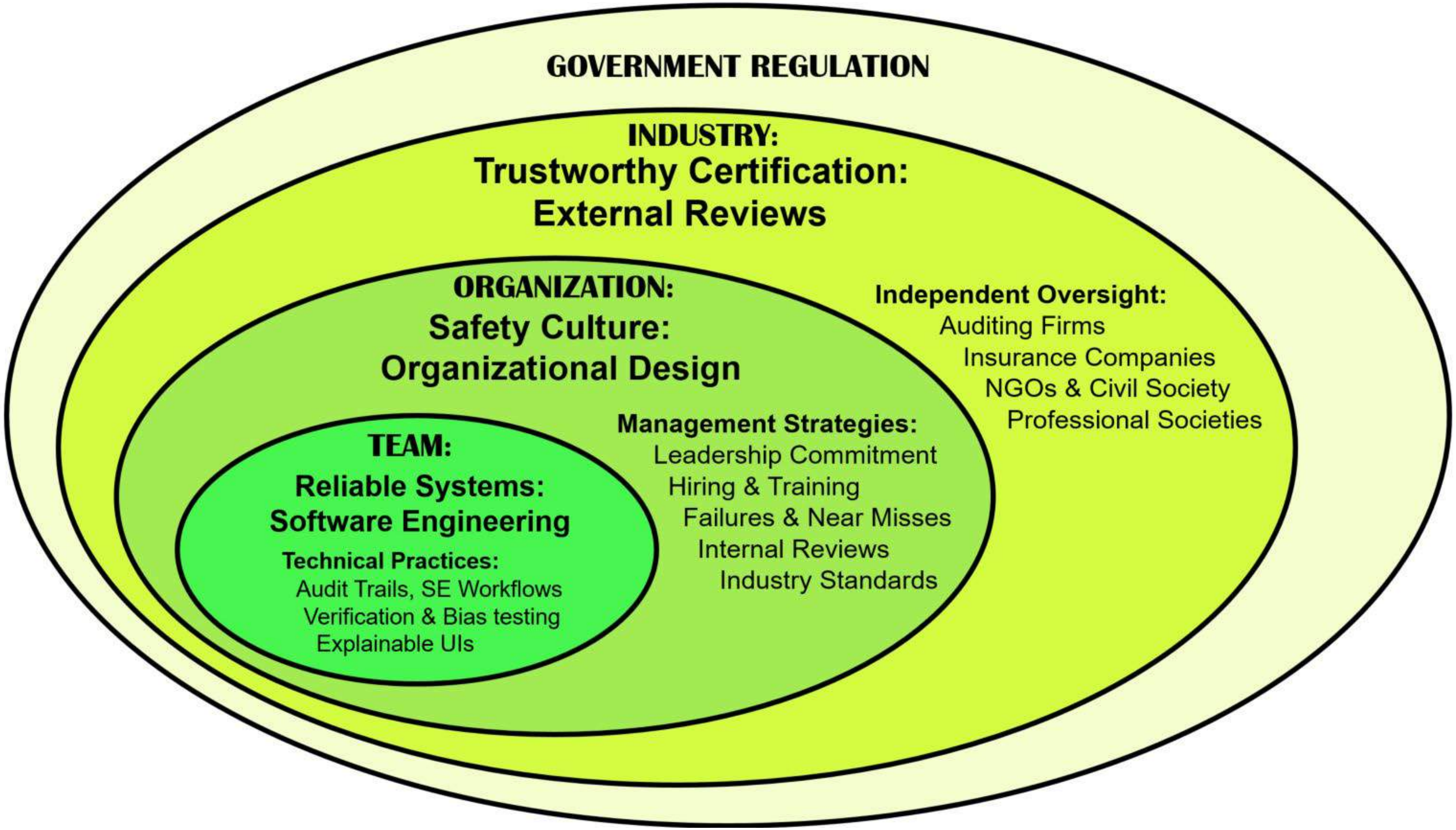
https://www.davincisurgery.com/

Bloomberg Terminal

Hospital Control Center

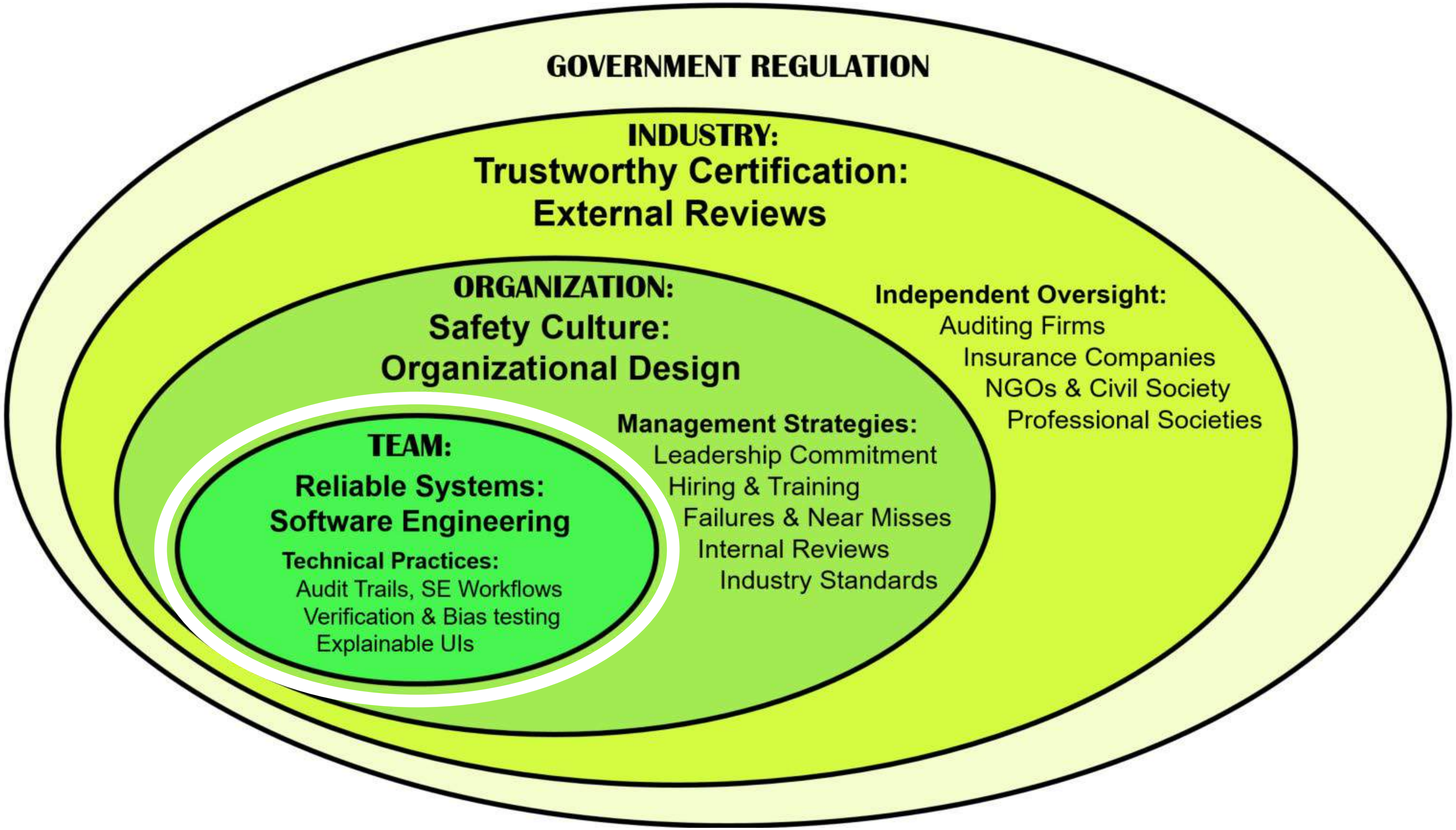
Counter Terrorism Center

Governance Structures for Human-Centered AI



ACM TIIS (Oct 2020) `https://dl.acm.org/doi/10.1145/3419764`

Governance Structures for Human-Centered AI



ACM TIIS (Oct 2020) `https://dl.acm.org/doi/10.1145/3419764`

TEAM

Reliable systems based on software engineering practices

1) Audit trails and analysis tools
2) Software engineering workflows
3) Verification & validation testing
4) Bias testing to improve fairness
5) Explainable user interfaces

TEAM

Reliable systems based on software engineering practices

1) Audit trails and analysis tools
2) Software engineering workflows
3) Verification & validation testing
4) Bias testing to improve fairness
5) Explainable user interfaces

Reliable Systems

Software engineering practices for a TEAM

1) Audit trails and analysis tools

"Flight Data Recorder for Every Robot"

- Retrospective analysis of failures
  - Understanding near misses
- Analysis to support preventive maintenance

Reliable Systems

Software engineering practices for a TEAM

5) Explainable user interfaces

- Retrospective explanations (local & global)

New Goal: **Prevent** confusion and surprise -

Prospective user interfaces

- Interactive, visual, exploratory

Mortgage Loan Explanations

Post-hoc Report

Enter amounts to request mortgage:

Mortgage amount requested	375000
Household monthly income	7000
Liquid assets	48000

Submit

Mortgage Loan Explanations

Post-hoc Report

Enter amounts to request mortgage:

Mortgage amount requested	375000
Household monthly income	7000
Liquid assets	48000

Submit

Enter amounts to request mortgage:

Mortgage amount requested	375000
Household monthly income	7000
Liquid assets	48000

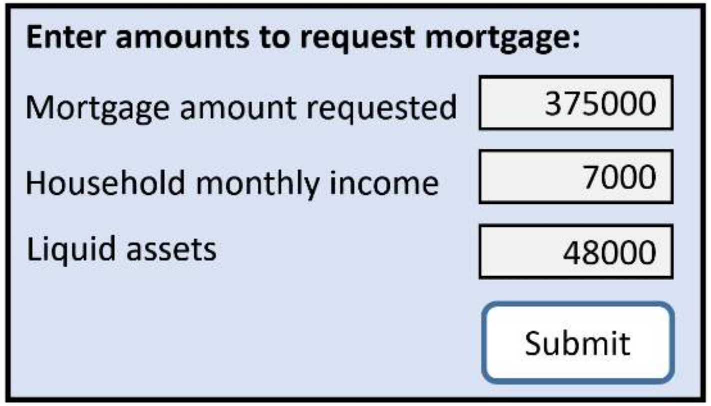
Submit

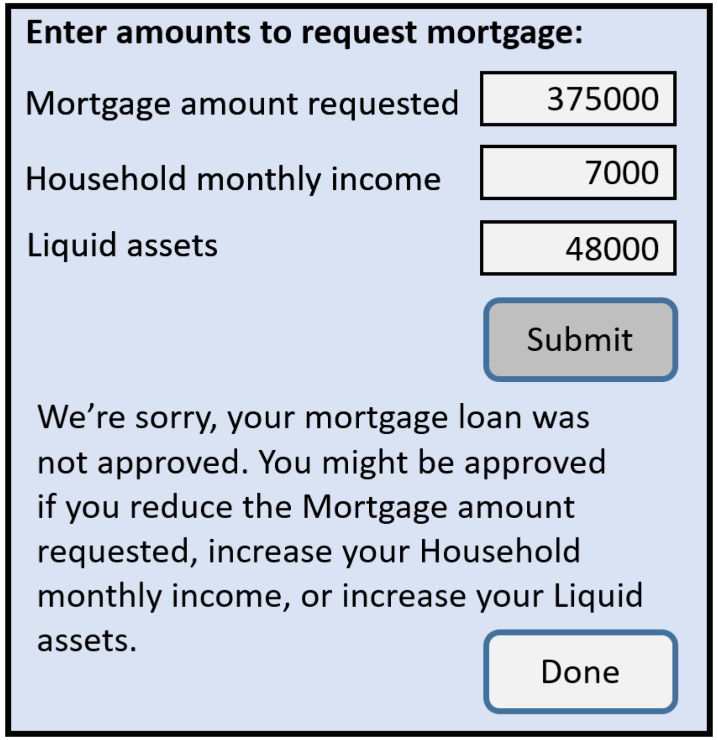
We're sorry, your mortgage loan was not approved. You might be approved if you reduce the Mortgage amount requested, increase your Household monthly income, or increase your Liquid assets.

Done

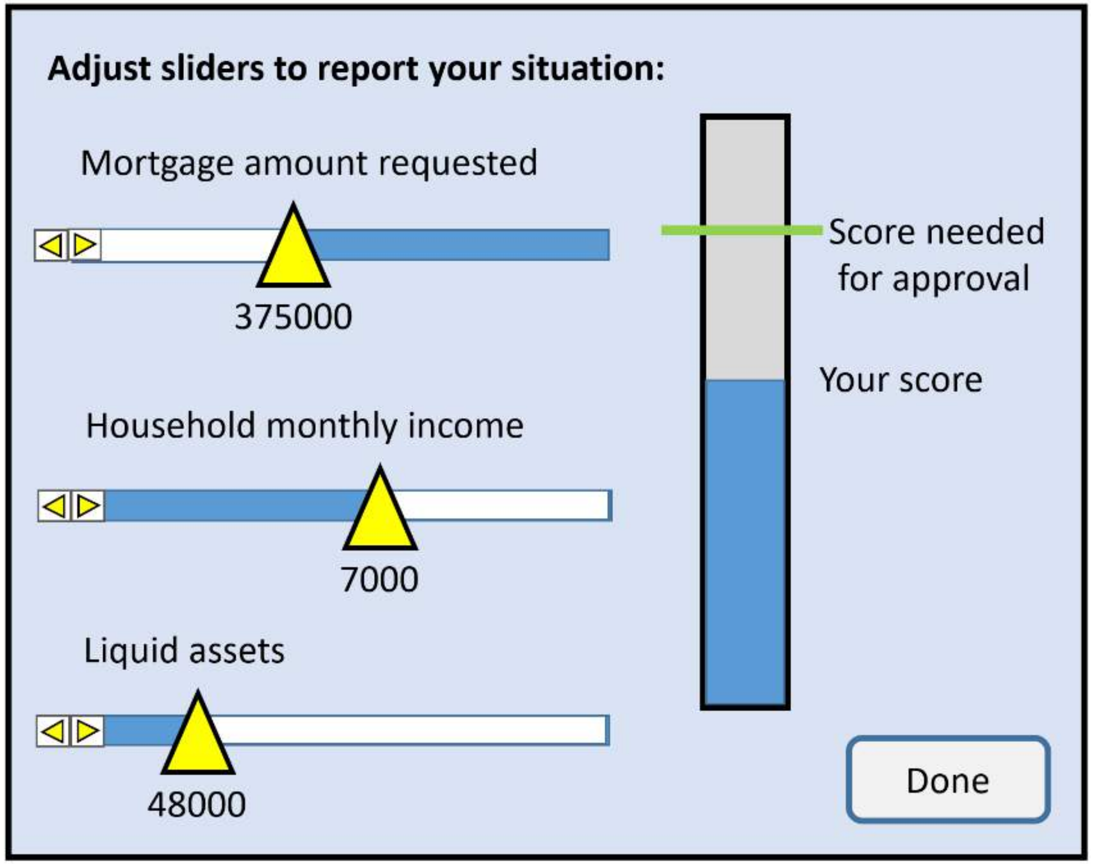
Mortgage Loan Explanations

Post-hoc Report

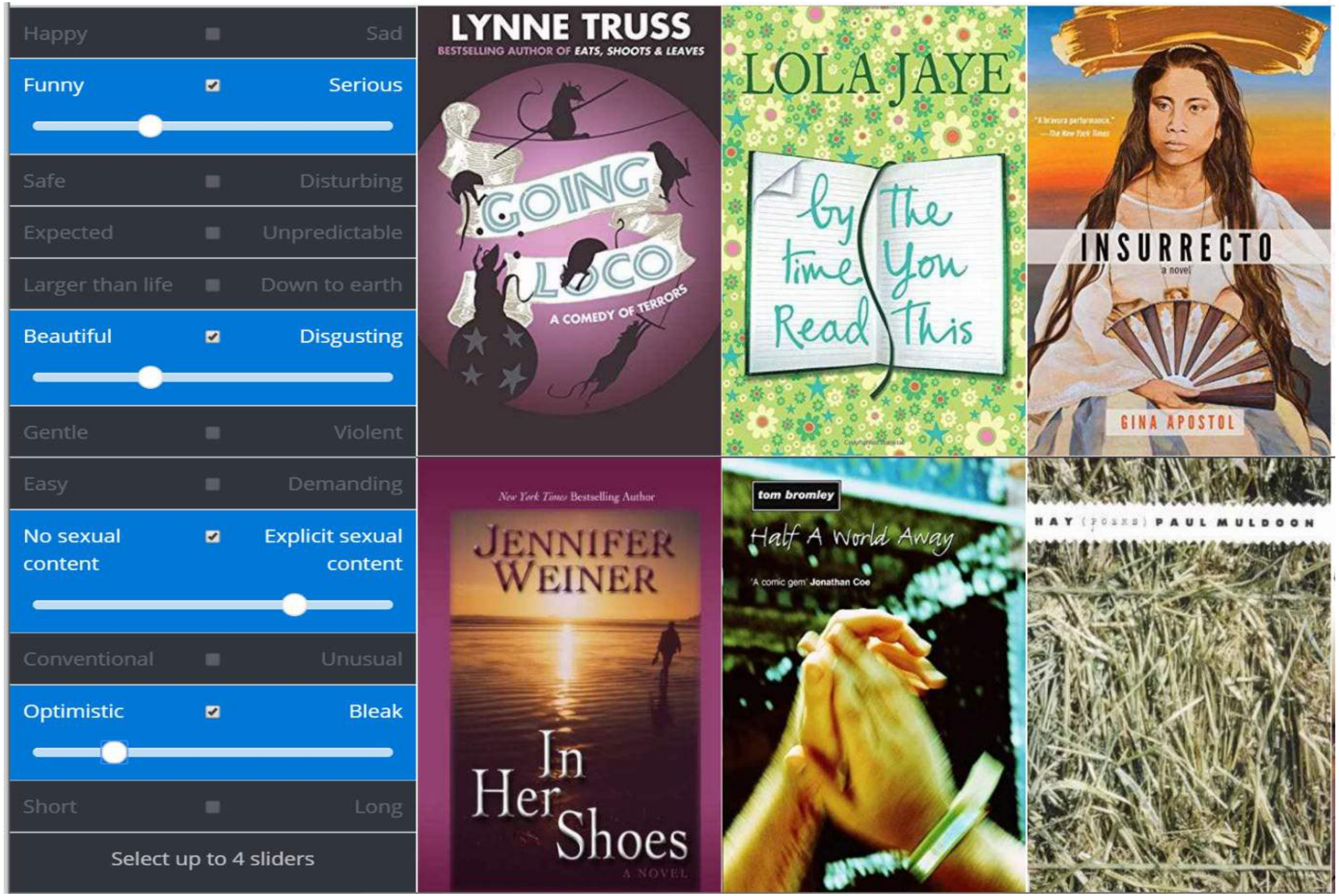




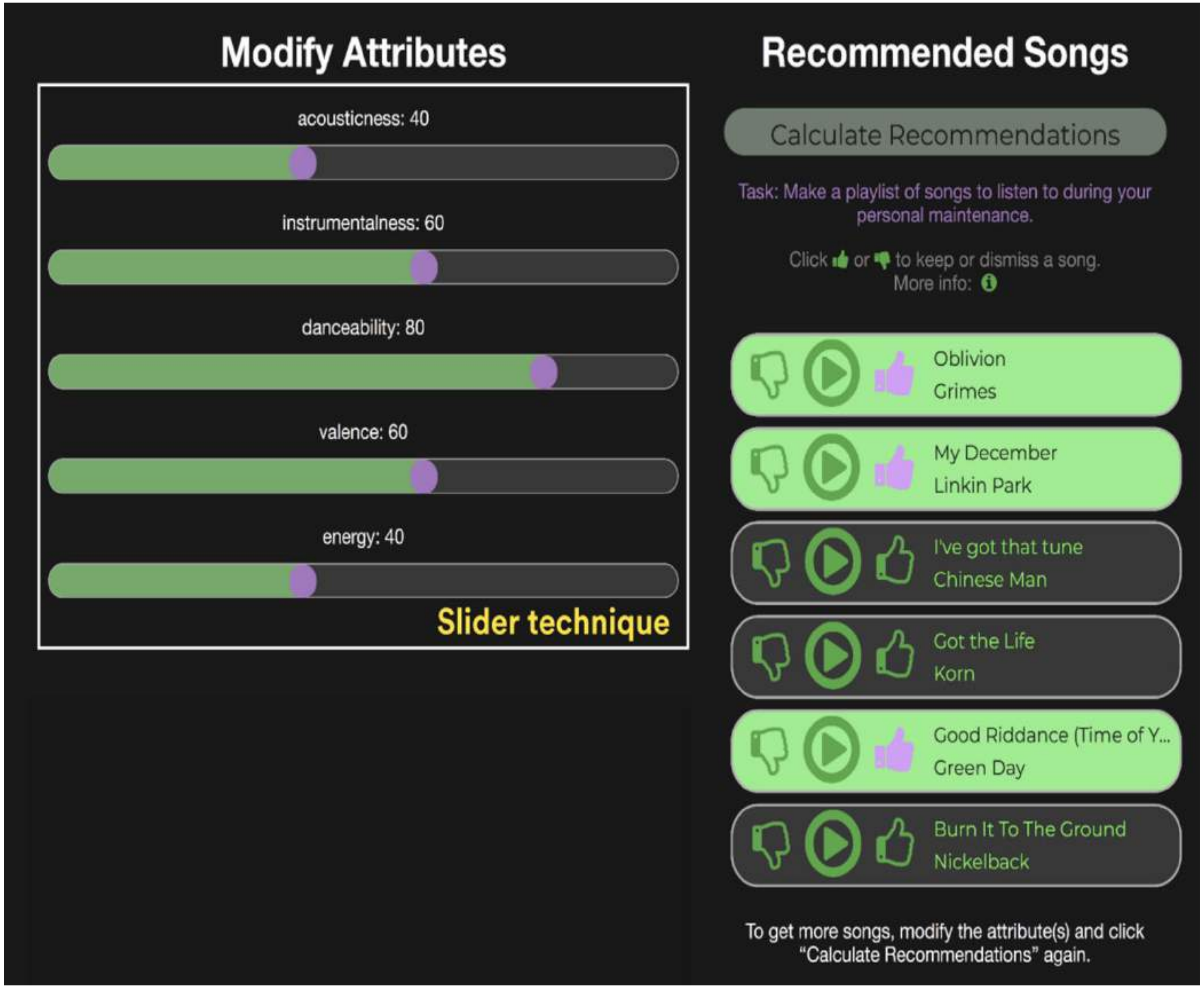
Prospective User Interface



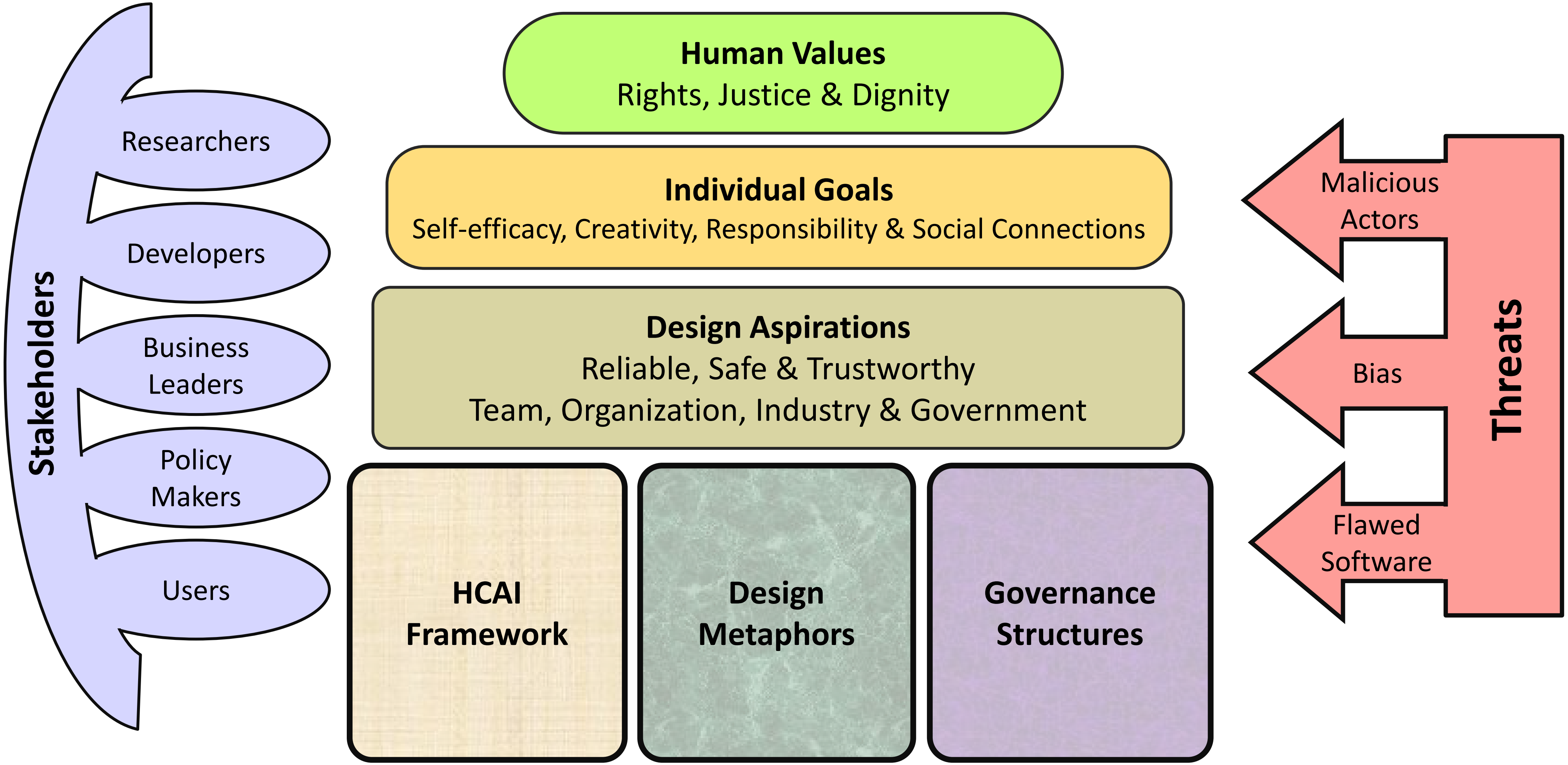
Recommenders: Whichbook.net



Recommender Control Panels

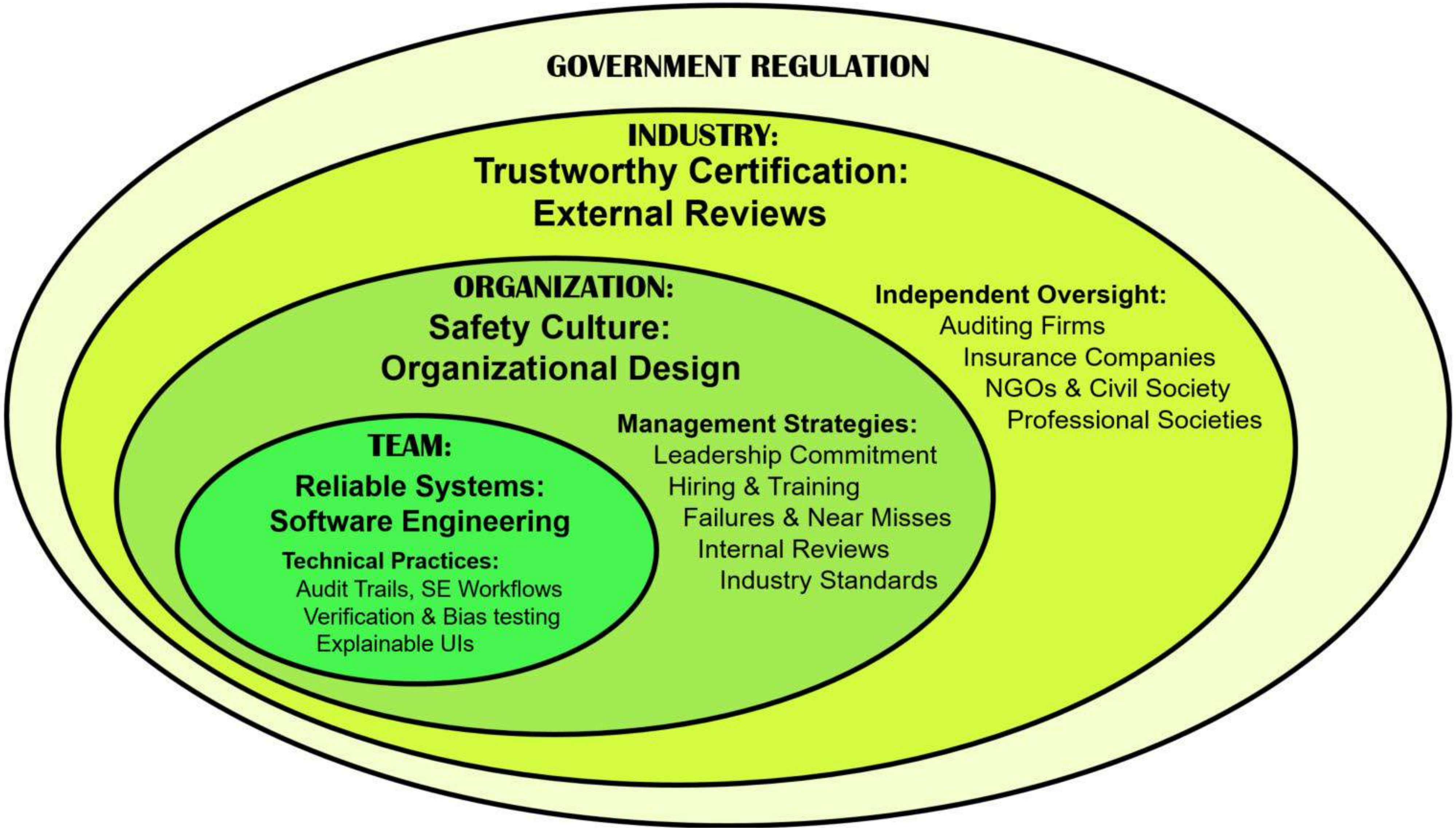


Human-Centered AI



Oxford University Press (Early 2022) `https://hcil.umd.edu/human-centered-ai/`

Governance Structures for Human-Centered AI



ACM TIIS (Oct 2020) `https://dl.acm.org/doi/10.1145/3419764`

Human-Centered Artificial Intelligence: Reliable, safe & trustworthy, *International Journal of Human-Computer Interaction 36,* 6 (March 2020). https://doi.org/10.1080/10447318.2020.1741118

Design lessons from AI's two grand goals: Human emulation and useful applications, *IEEE Transactions on Technology & Society 1,* 2 (June 2020). https://ieeexplore.ieee.org/document/9088114

Bridging the gap between ethics and practice: Guidelines for reliable, safe, and trustworthy Human-Centered AI systems, *ACM Trans. on Interactive Intelligent Systems 10,* 4 (Oct 2020). https://dl.acm.org/doi/10.1145/3419764

Human-Centered Artificial Intelligence: Three fresh ideas, *AIS Trans. on Human-Computer Interaction 12,* 3 (Oct 2020). https://aisel.aisnet.org/thci/vol12/iss3/1/

Human-Centered AI, *NAS ISSUES 37, 2* (Winter 2021). https://issues.org/human-centered-ai/

Summary & resources: https://hcil.umd.edu/human-centered-ai/

The Future is Human-Centered

Google Group

`https://groups.google.com/g/human-centered-ai`

Twitter Account

`@HumanCenteredAI`

Website

`https://hcai.site`

The Future is Human-Centered

Torrey Mortenson, INL

June 8, 2021

Designing Explainable AI

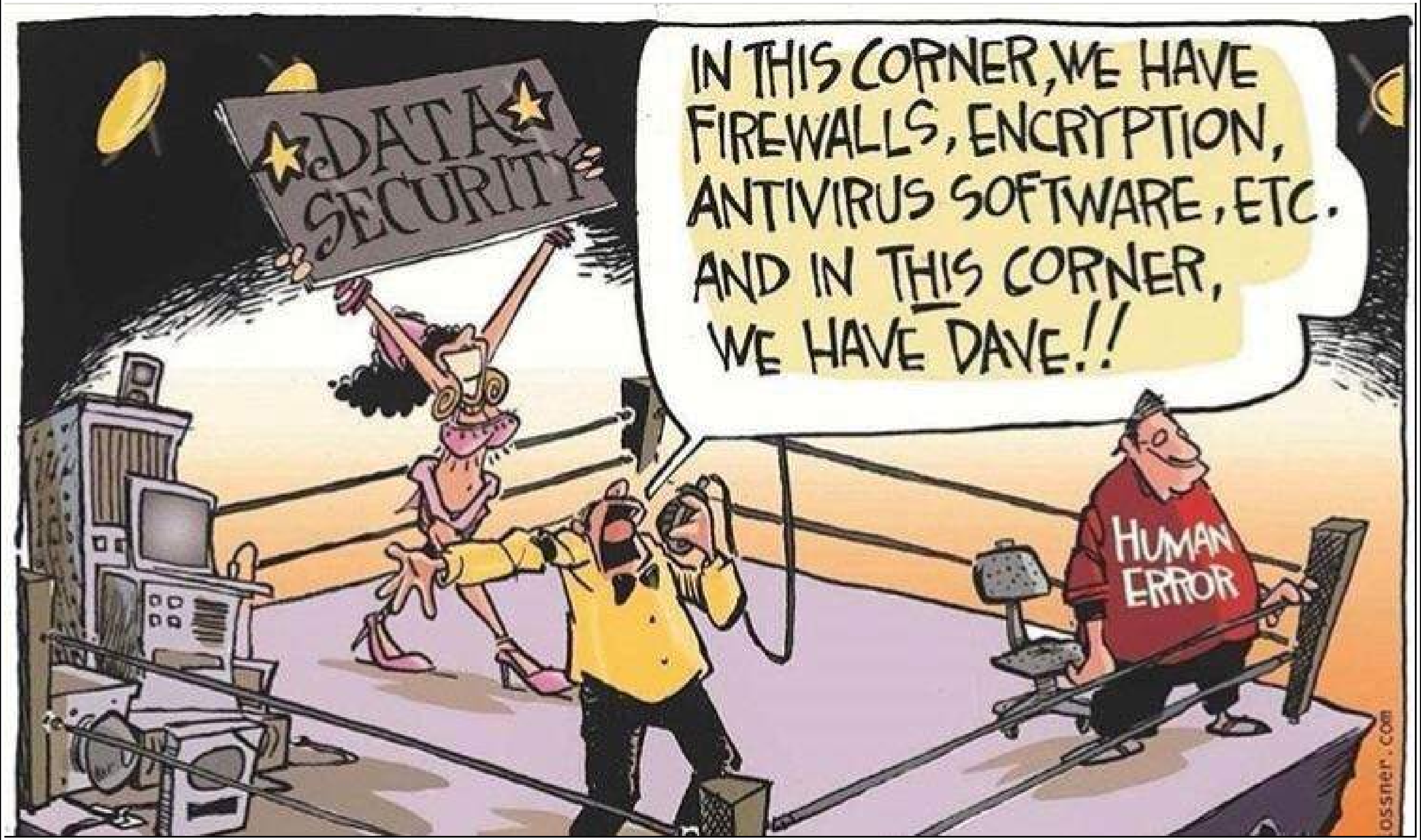
Idaho National Laboratory

Why do we need to design explainable ML/AI?

- Because of its application to things that matter.
  - Critical infrastructure instead of cereal selection
- ML/AI is inscrutable at scale
  - We don’t really understand in a fundamental way how these algorithms work. (Mickens, 2018)
- Stochasticity isn’t a good explanation, e.g. gradient descent

¯_(ツ)_/¯

- Dr. James Mickens, 2018 Usenix Security Keynote. *"Q: Why Do Keynote Speakers Keep Suggesting That Improving Security Is Possible?*
  A: Because Keynote Speakers Make Bad Life Decisions and Are Poor Role Models"



Designing for inscrutability – Role of Human Centered design

Human Centered Design from day one

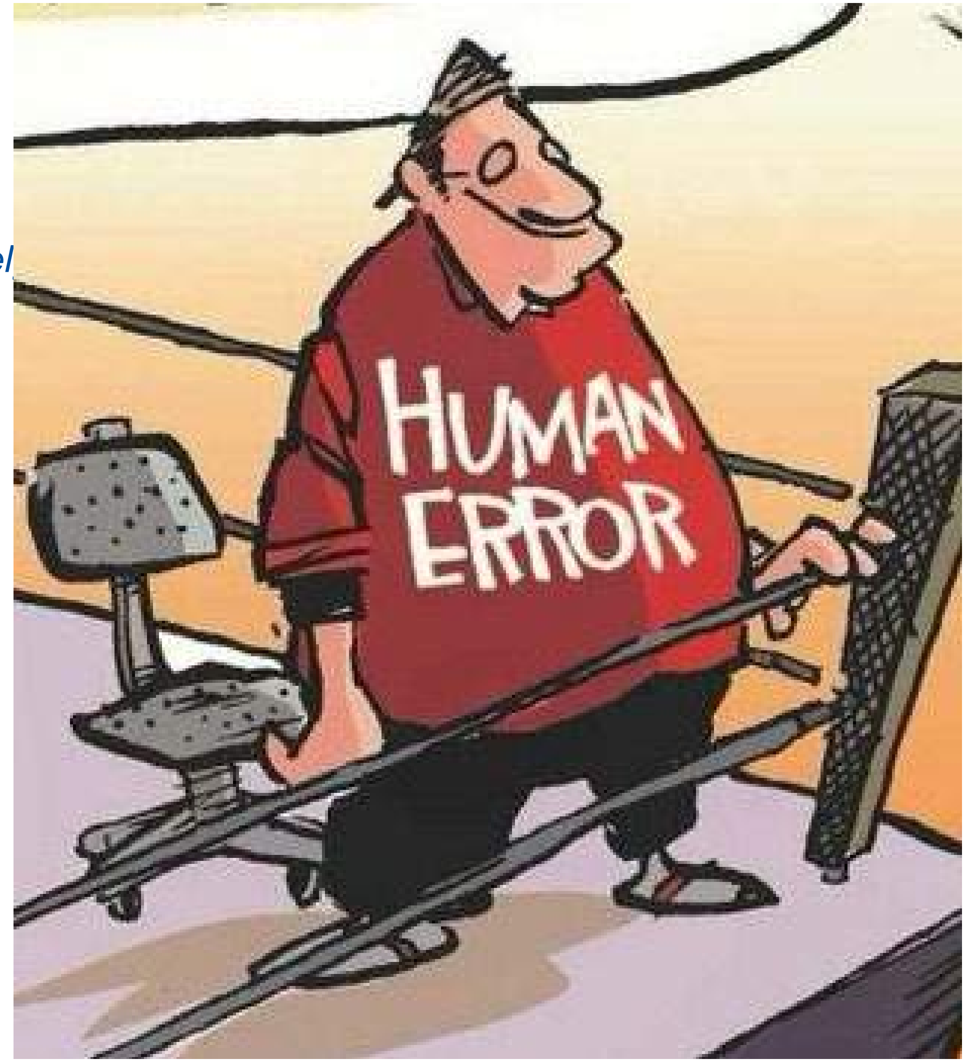
- Involvement of human factors is critical
  - Model implications
  - Measure implications
  - Every aspect of the model needs to be explainable.
    - Impossible to predict what may need to be explained.

- **Why human factors?**
  - **AI/ML is often an inscrutable black box, do you know what else is an inscrutable black box?**

Dave!

- *Any resemblance to any "Daves" living or dead is purel*

- Your HF colleagues have spent their career understanding and designing for Daves
- Designing for inscrutability is human factors at its core
- Late or no involvement of HF ***will*** lead to an AI/ML algorithm that is not transparent, explainable, or trustworthy and therefore unfit for use in critical human infrastructure



Predictive maintenance project

- Predicting the health of a circulating water pump
  - XAI/HCAI as communication
  - What if we could only talk to the model?

"How do you know?"

"What is specifically wrong?"

"Are you sure?"

"How 'unhealthy' – how bad is it doc?"

Health of Pump

Unhealthy

"Which sensors are you seeing?"

"What should we do?"

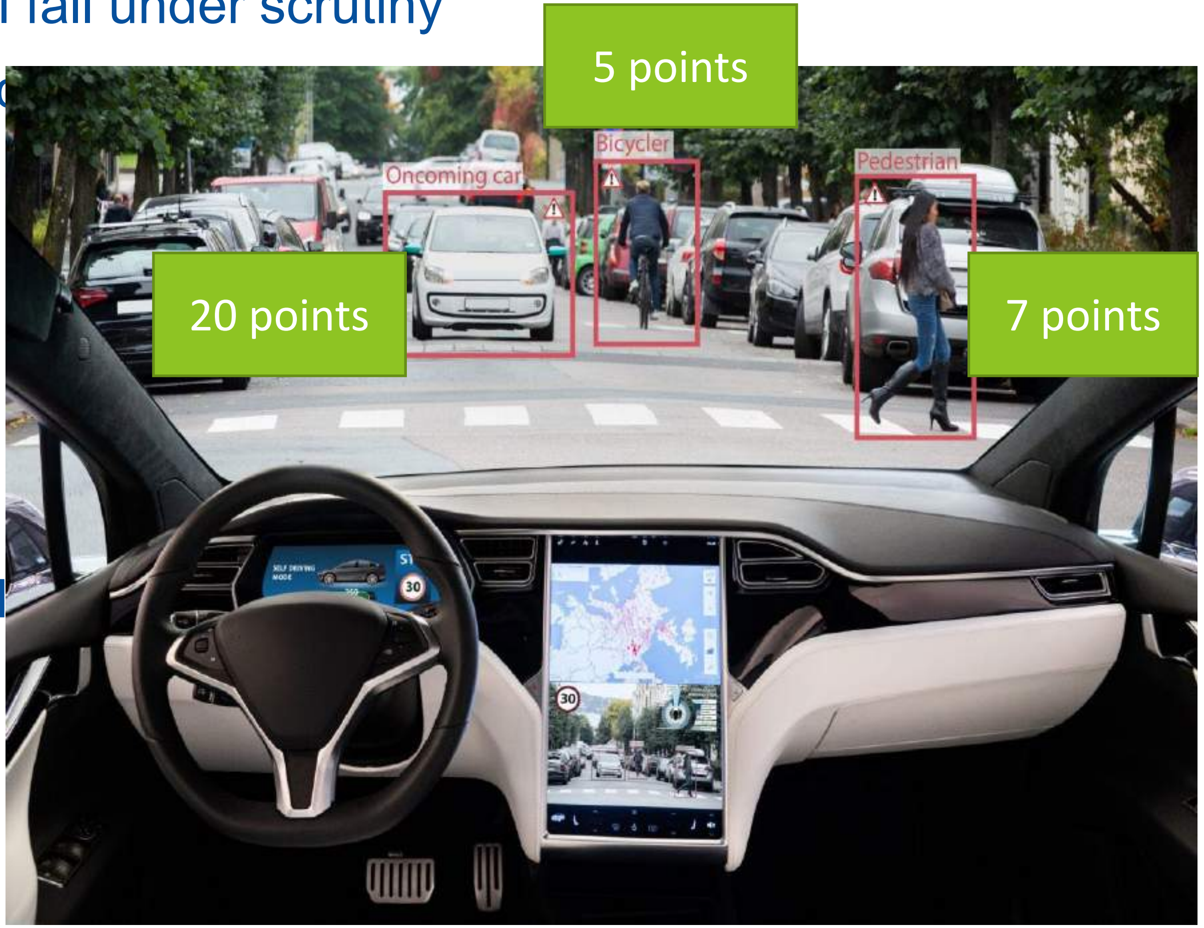
Can the model answer these? Clearly, precisely, and verifiably?

Predictive maintenance project (cont.)

- HF researchers worked closely with the model development team to shape the specific user questions that the model needed to support
- Your ultimate visualization and display has to support the aspects of explainability
- By working with modelers, we were able to explore different methods of interpretability like SHAP, feature interaction, and feature importance.
- Currently in the process of testing prototype visualization with users and will have feedback on adjustments to the model moving forward

Designing for trust, and failure

- AI/ML algorithms will fail and will fall under scrutiny
- Consider how to explain the mod
  - Regulators
  - Policy makers
  - The courts
  - Operators
  - Lay people
  - Communities
- When it fails, what does it do? H



Idaho National Laboratory

Explainable Dimensionality Reduction Using Scientific Constraints

Ramakrishnan Kannan
Group Lead, Discrete Algorithms
https://ramkikannan.github.io
https://github.com/ramkikannan
https://ramkikannan.github.io/planc-api

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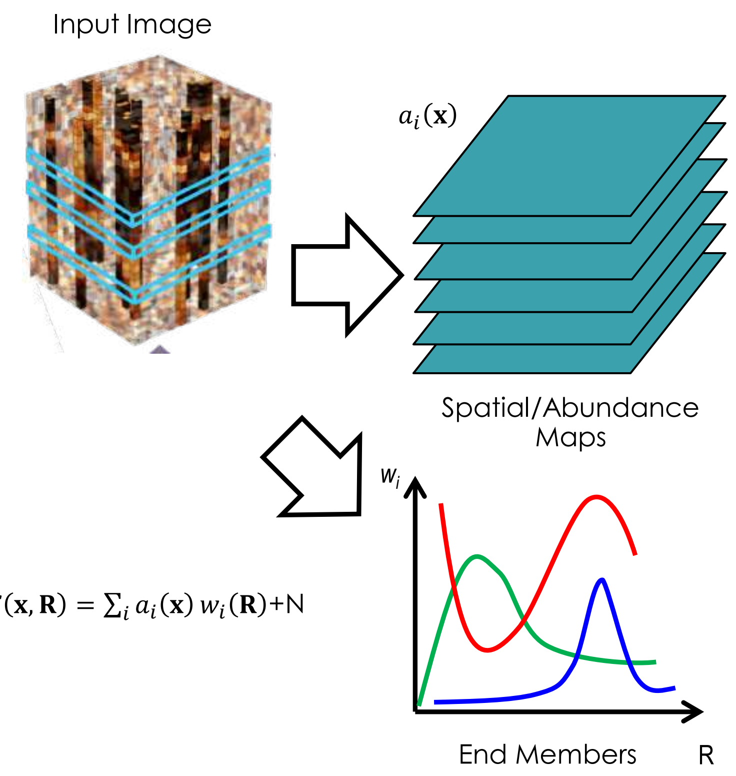
- Students - Srinivas Eswar (GATech), Koby Hayashi(Wake Forest), Jeff Graves (TNTech), Rina Singh(TNTech), Mosharraf Hossain (TNTech), Luna Xu (VATech), Sekeong Hong (NCSU), Euna Kim(GATech), Seema Chouhan(UMASS), Mark Heimann(Umich), Pravallika Devineni (UCR), Thomas Blum(UCI)

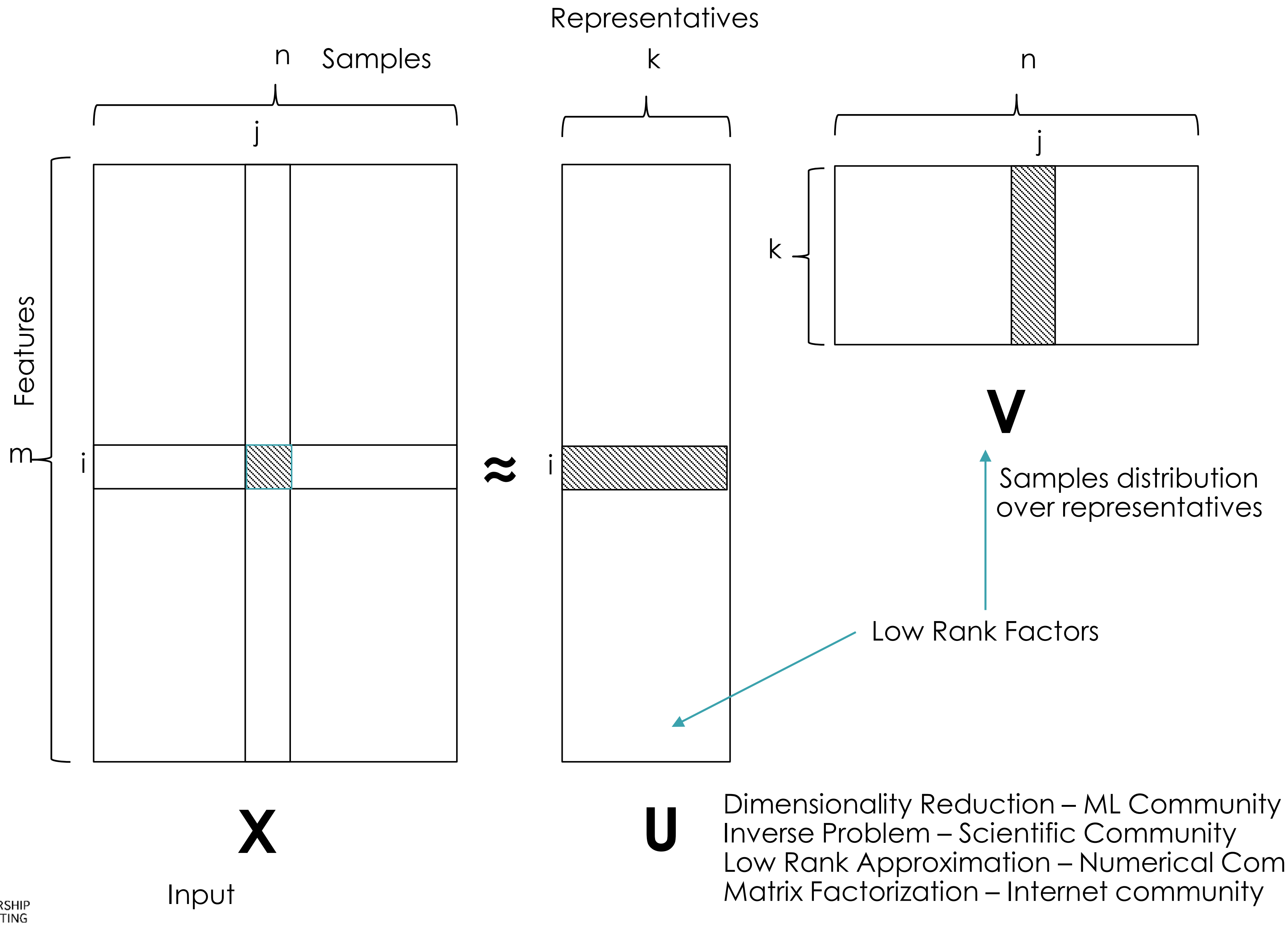
Unmixing

- Understanding terrestrial information in an unknown place from satellite images
- Identifying presence of hidden unknown/foreign bodies in a scanned image - Eg., contamination in food articles, camouflaged explosives etc.
- Biological application - spectral karyotyping, immunofluorescence, live-cell imaging, drug discovery, and tissue pathology – Eg., Unmixing on Spectral imaging of the stained tissues using multiple dyes.
- Physics and Material Sciences – Mapping properties to end-members. Comparing different materials



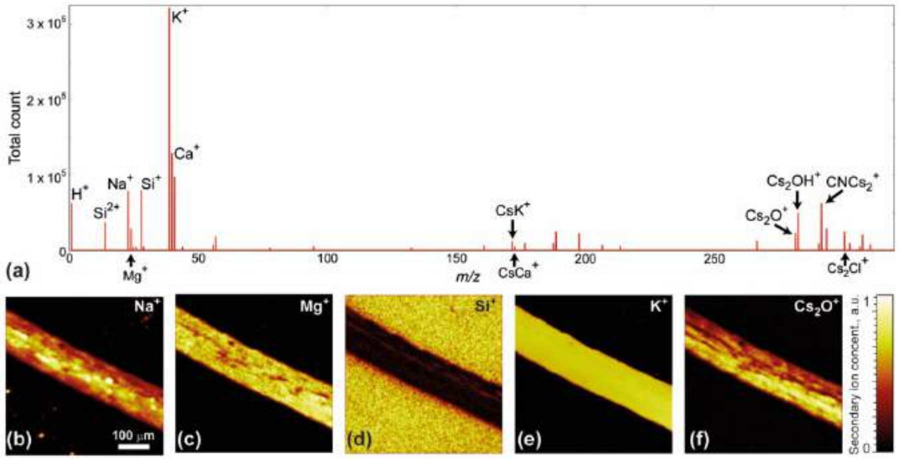
$S(\mathbf{x},\mathbf{R}) = \sum_i a_i(\mathbf{x})\, w_i(\mathbf{R})$+N

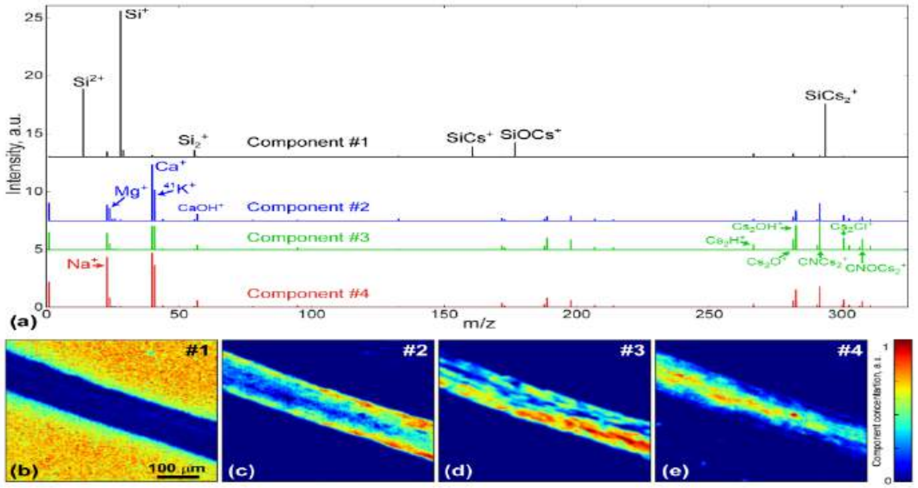
Matrix Factorization (MF)

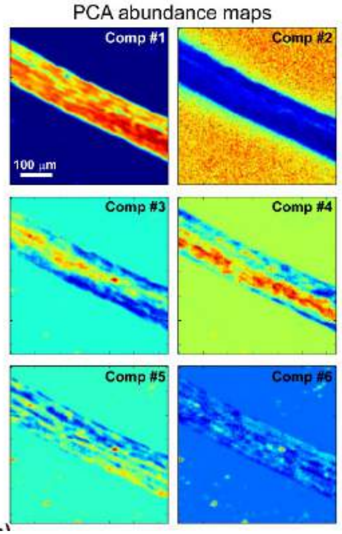


Dimensionality Reduction – ML Community
Inverse Problem – Scientific Community
Low Rank Approximation – Numerical Community
Matrix Factorization – Internet community

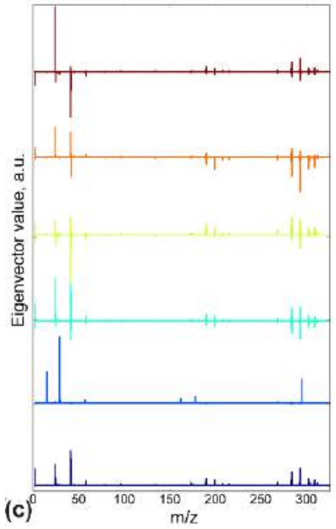
Example 1 : NMF vs. PCA







PCA Eigen vectors



Both PCA and NMF are insufficient
They do not consider the neighbourhood information
To consider this information, we use regularization

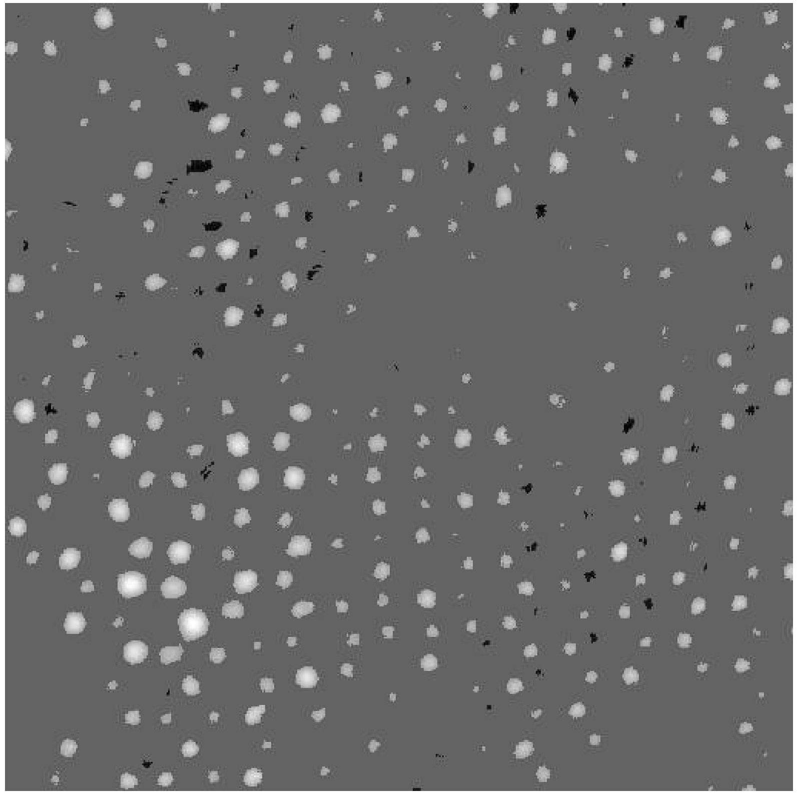
Atomic Motion of MoSe2 – (https://smc-datachallenge.ornl.gov)

Zhou, T. and D. Tao (2011). Godec: Randomized low-rank & sparse matrix decomposition in noisy case. International conference on machine learning, Omnipress.

$$\min_{L,S} \left|\left|A - L - S\right|\right|_F^2$$

subject to

$$rank(L) \leq r;\ card(S) \leq k$$



Symmetric NMF

$$\min_{\mathbf{H}\geq 0} \|\mathbf{A}-\mathbf{H}\mathbf{H}^{\mathsf{T}}\|_F^2.$$

- ANLS Variant $\min_{\{\mathbf{W},\mathbf{H}\}\geq 0} \|\mathbf{A}-\mathbf{W}\mathbf{H}^{\mathsf{T}}\|_F^2 + \gamma\|\mathbf{W}-\mathbf{H}\|_F^2.$ $\quad \min_{\mathbf{H}\geqslant 0} \left\| \begin{bmatrix} \mathbf{W} \\ \sqrt{\gamma}\mathbf{I}_k \end{bmatrix} \mathbf{H}^{\mathsf{T}} - \begin{bmatrix} \mathbf{A} \\ \sqrt{\gamma}\mathbf{W}^{\mathsf{T}} \end{bmatrix} \right\|_F^2,$
- Gauss Newton based Conjugate Gradient
  - Computing Gradient
  - Applying Gramian of Jacobian

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} + \operatorname*{argmin}_{\mathbf{p}} \left\| \mathbf{J}^{(t)}\mathbf{p} + \mathbf{r}^{(t)} \right\|_2^2.$$

Algorithm 2 $[\mathbf{W},\mathbf{H}] = \text{SymGNCG}(\mathbf{A},k,s_{\max})$

Require: $\mathbf{A} \in \mathbb{R}_+^{n\times n}$ is distributed across a $\sqrt{p}\times\sqrt{p}$ grid of processors, $k>0$ is rank of approximation, p divides n
Require: Local matrices: $\mathbf{H}_{ij},\mathbf{X}_{ij},\mathbf{P}_{ij},\mathbf{R}_{ij},\mathbf{Y}_{ij}$ are $n/p\times k$

```
Proc p_ij initializes H_ij
while stopping criteria not satisfied do
    X = 0                                   % Initialize x_0 = 0
    R = Compute-Gradient(A,H)               % r = b − J^T J x_0
    p_ij sets P_ij = R_ij                   % p = r
    p_ij computes ε_ij^old = ⟨R_ij, R_ij⟩
    compute ε^old = Σ_{i,j} ε_ij^old using all-reduce across all procs
    for s = 1 to s_max do
        Y = Apply-Gramian(H,P)              % y = J^T J p
        p_ij computes α_ij = ε^old / ⟨P_ij, Y_ij⟩
        compute α = Σ_{i,j} α_ij using all-reduce across all procs
        p_ij computes X_ij = X_ij + αP_ij   % x = x + αp
        p_ij computes R_ij = R_ij − αY_ij   % r = r − αy
        p_ij computes ε_ij = ⟨R_ij, R_ij⟩
        compute ε = Σ_{i,j} ε_ij using all-reduce across all procs
        p_ij computes P_ij = R_ij + (ε/ε^old) P_ij   % p = r + βp
        ε^old = ε
    end for
    p_ij computes H_ij = [H_ij − X_ij]_+    % projected GN step
end while
```

Ensure: $\mathbf{H} \approx \operatorname*{argmin}_{\tilde{\mathbf{H}}\geqslant 0} \|\mathbf{A}-\tilde{\mathbf{H}}\tilde{\mathbf{H}}^{\mathsf{T}}\|_F^2$
Ensure: $\mathbf{H}$ is $n\times k$ row-wise distributed across processors

(a) Original Image (b) Boundary Map (c) Segmented Image

Fig. 13. Boundary detection and image segmentation using features generated by SymNMF.

TABLE I
PER-ITERATION PER-PROCESSOR COSTS FOR DENSE CASE

Algorithm	flops	words	messages
ANLS	$\frac{4n^2k}{p}+O(\frac{nk^2}{p})$	$O(\frac{nk}{\sqrt{p}}+k^2)$	$O(\log p)$
GNCG	$\frac{2n^2k}{p}+O(\frac{s_{\max}nk^2}{p})$	$O(\frac{nk}{\sqrt{p}}+s_{\max}k^2)$	$O(s_{\max}\log p)$

S. Eswar, K. Hayashi, G. Ballard, R. Kannan, H. Park and R. Vuduc: Distributed-Memory Parallel Symmetric Non-negative Matrix Factorization. Accepted at SC'20

Hierarchical Non-negative Matrix Factorization

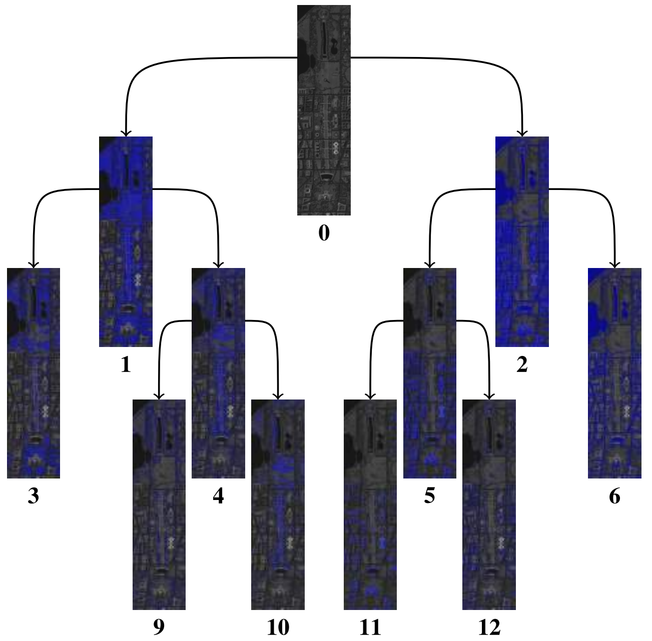
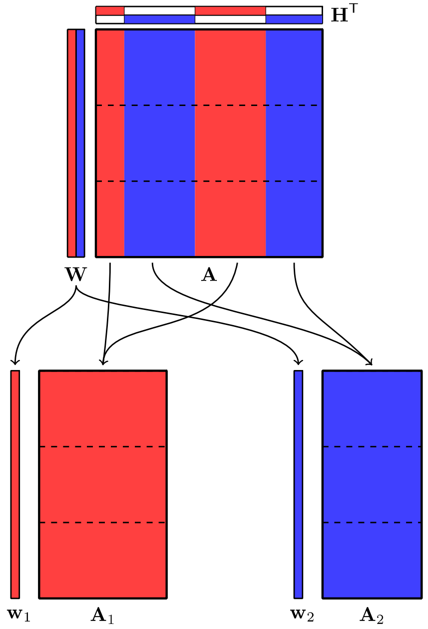


Figure 1: Hierarchical Clustering of DC Mall HSI



$$\min_{\bar{h}_{i,1},\bar{h}_{i,2}\geqslant 0}\left\|\begin{bmatrix}\mathbf{w}_1 & \mathbf{w}_2\end{bmatrix}\begin{bmatrix}\bar{h}_{i,1}\\ \bar{h}_{i,2}\end{bmatrix}-\mathbf{a}_i\right\| = \min_{\bar{h}_{i,1},\bar{h}_{i,2}\geqslant 0}\left\|\bar{h}_{i,1}\mathbf{w}_1+\bar{h}_{i,2}\mathbf{w}_2-\mathbf{a}_i\right\|$$

Recursively solve a Rank-2 NMF

Algorithm 2 Hierarchical Clustering [15]

Require: $\mathbf{A}$ is $m \times n$, k is target number of leaf clusters
function $\mathcal{T} = $ HIER-R2-NMF($\mathbf{A}$)
  $\mathcal{R} = $ node($\mathbf{A}$) *% create root node*
  SPLIT($\mathcal{R}$)
  inject($\mathcal{Q}$,$\mathcal{R}$.left) *% create priority queue*
  inject($\mathcal{Q}$,$\mathcal{R}$.right) *% of frontier nodes*
  while size($\mathcal{Q}$) $< k$ **do**
    $\mathcal{N} = $ eject($\mathcal{Q}$) *% frontier node with max score*
    SPLIT($\mathcal{N}$.left) *% split left child*
    inject($\mathcal{Q}$,$\mathcal{N}$.left) *% and add to $\mathcal{Q}$*
    SPLIT($\mathcal{N}$.right) *% split right child*
    inject($\mathcal{Q}$,$\mathcal{N}$.right) *% and add to $\mathcal{Q}$*
  end while
end function
Ensure: $\mathcal{T}$ is binary tree rooted at $\mathcal{R}$ with k frontier nodes, each node has subset of cols of $\mathbf{A}$ and feature vector $\mathbf{w}$

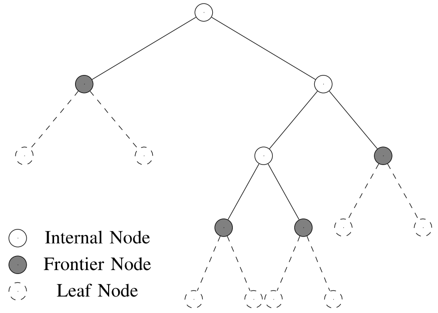
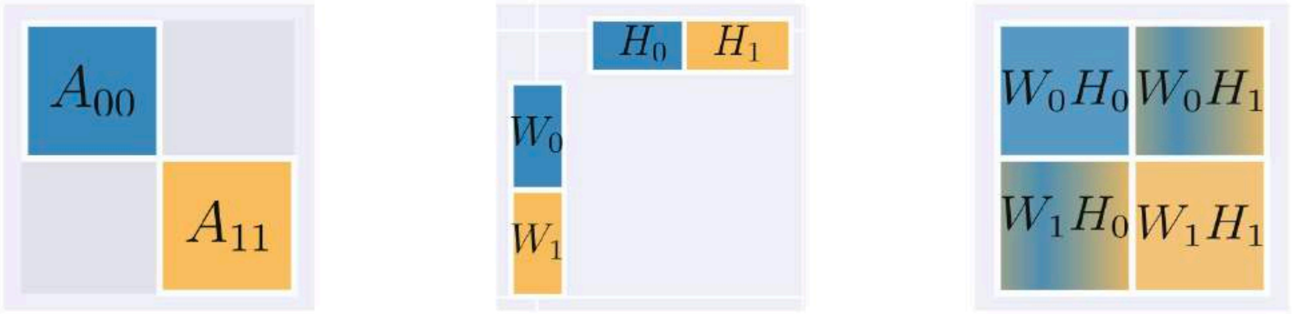
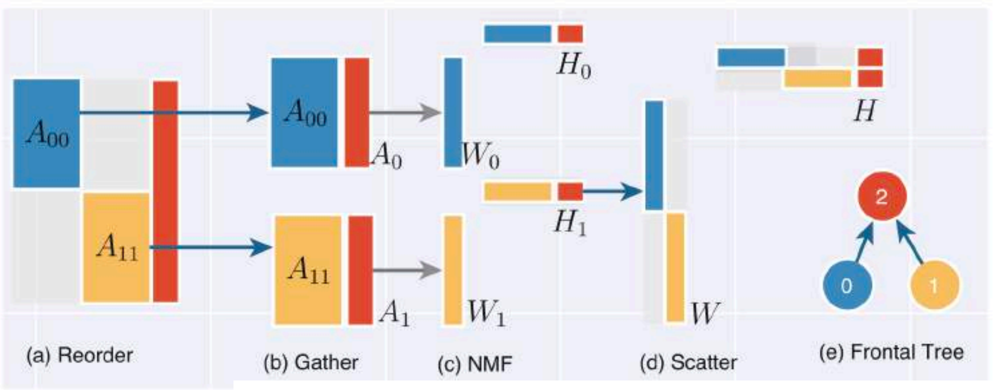


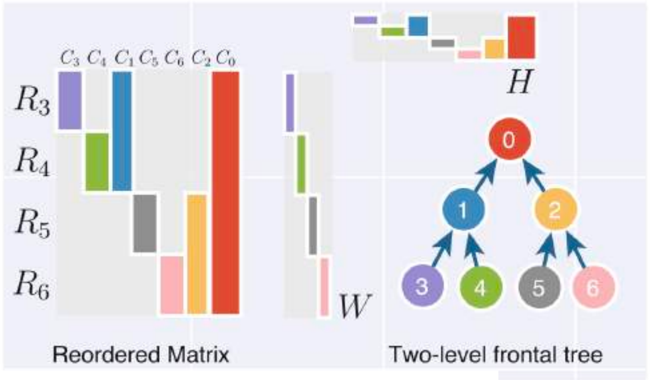
Figure 2: Hierarchy node classification

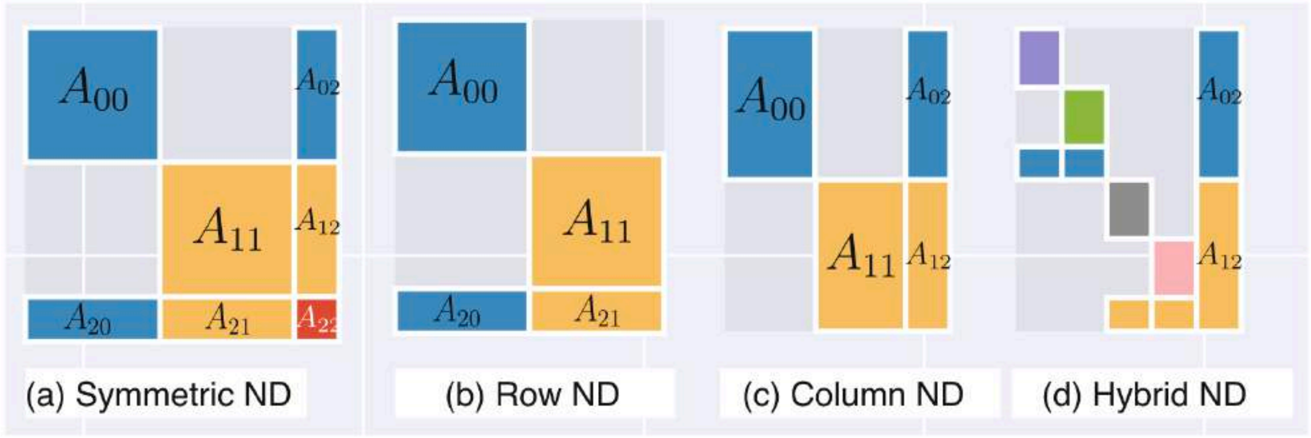
L. Manning, G. Ballard, R. Kannan, H. Park: Parallel Hierarchical Clustering using Rank-Two Nonnegative Matrix Factorization. Communicated to HiPC'2020

Multifrontal NMF (MFNMF)







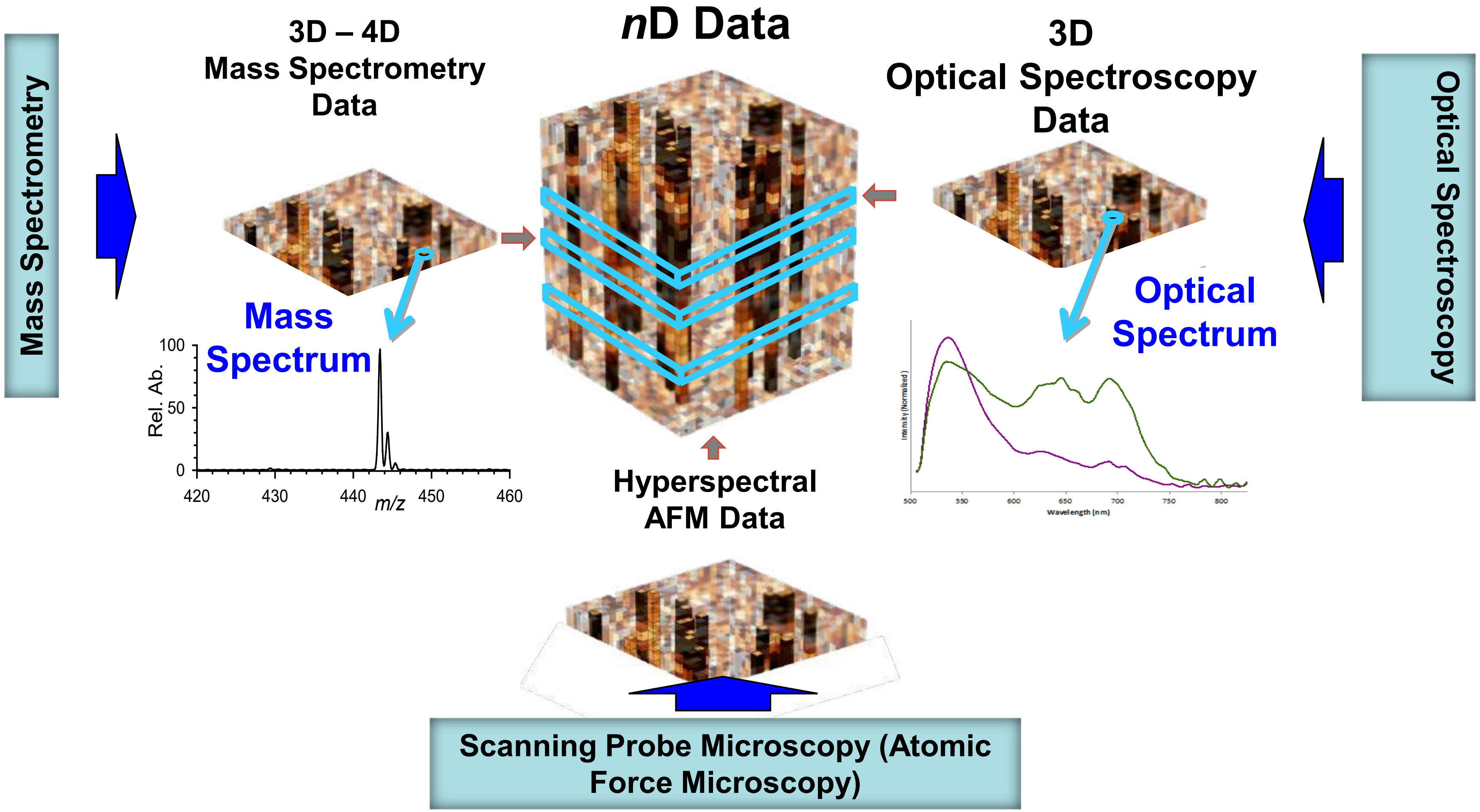


Piyush Sao, Ramakrishnan Kannan: **Multifrontal Non-negative Matrix Factorization.** PPAM (1) 2019: 543-554

Dense Tensor Factorization

Dimensionality Reduction in Scientific Data

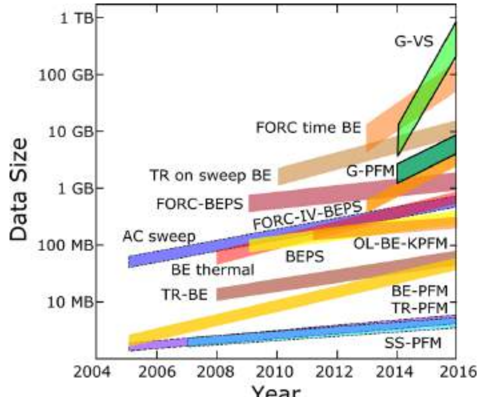
- Multimodal characterization of materials – *comprehensive characterization from chemical composition to functional properties on the nanoscale*



Thanks: Anton Ievlev

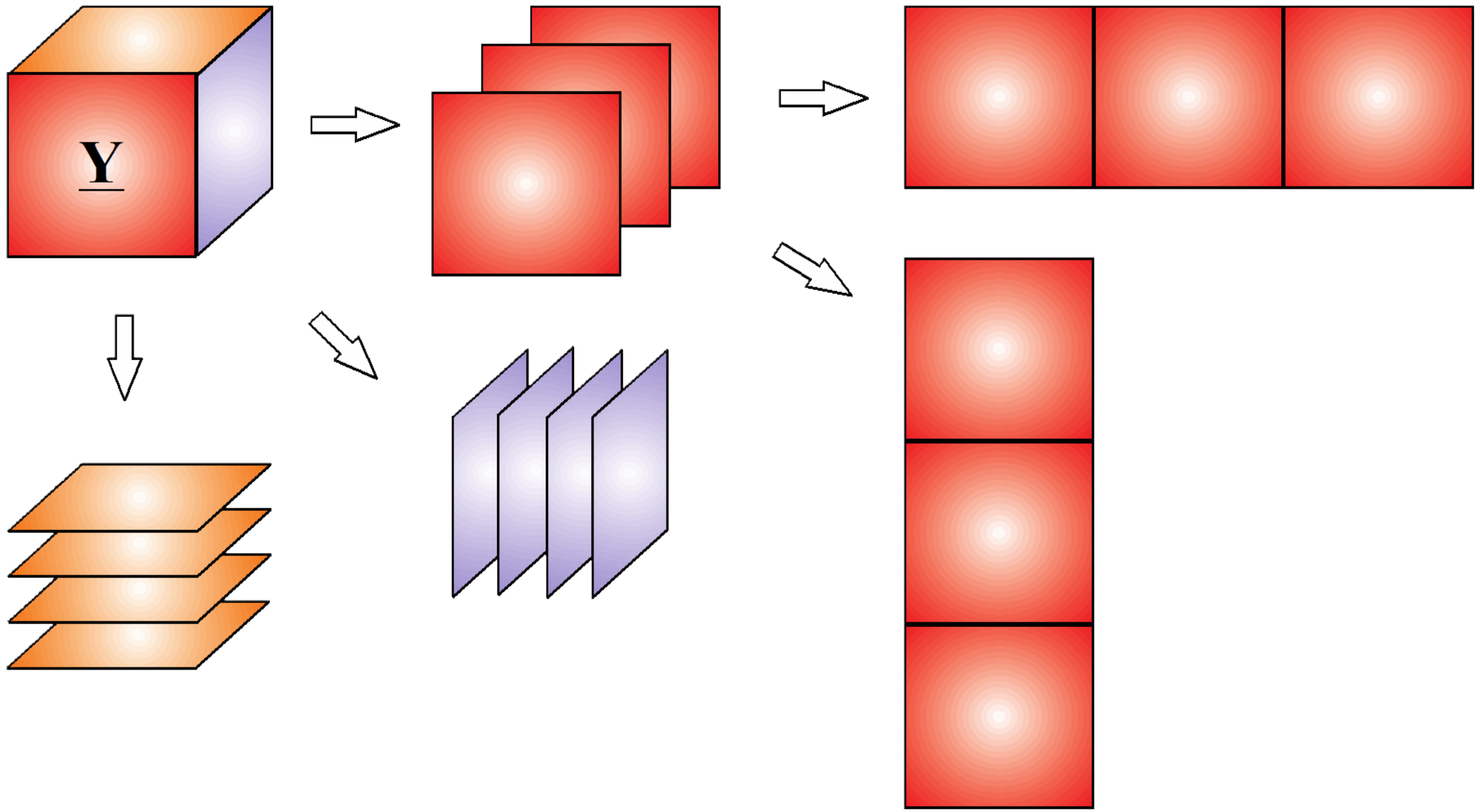
How Big? (Kalinin et.al., ACS Nano, 2016)

technique	dimensionality	target data set[a]	target data size[c]
band excitation piezoresponse force microscopy (BE-PFM)	3D, space and ω	$(256 \times 256) \times 64$	32 MB
switching spectroscopy PFM (SS-PFM)	3D, space and voltage	$(64 \times 64) \times 128$	4 MB
time relaxation PFM (TR-PFM)	3D, space and time	$(64 \times 64) \times 128$	4 MB
AC sweeps	4D, space, ω, voltage	$(64 \times 64) \times 64 \times 256$	512 MB
BE polarization switching (BEPS)	4D, space, ω, voltage	$(64 \times 64) \times 64 \times 128$	256 MB
BE thermal	4D, space, ω, temperature	$(64 \times 64) \times 64 \times 256$	512 MB
time relaxation BE (TR-BE)	4D, space, ω, time	$(64 \times 64) \times 64 \times 64$	64 MB
FORC BEPS	5D, space, ω, voltage, voltage	$(64 \times 64) \times 64 \times 64 \times 16$	2 GB
time relaxation on sweep, BE	5D, space, ω, voltage, time	$(64 \times 64) \times 64 \times 64 \times 64$	16 GB
FORC time BE	6D, space, ω, voltage, voltage, time	$(64 \times 64) \times 64 \times 64 \times 16 \times 64$	128 GB
FORC IV BEPS	5D, space, ω, voltage, cycle	$(64 \times 64) \times 64 \times 64 \times 16$	4 GB
FORC IV and FORC IV-Z	4D, space, voltage, cycle	$(64 \times 64) \times 64 \times 20$	200 MB
time-resolved Kelvin probe force microscopy (KPFM)	3D, space, time	$(60 \times 20) \times 1 \times 10^6$	8 MB
open loop (OL) BE KPFM	4D, space, ω, voltage	$(256 \times 256) \times 32 \times 16$	256 MB
general-mode PFM (G-PFM)	3D, space and voltage	$(256 \times 256) \times 1.6 \times 10^4$	4 GB
G-mode voltage spectroscopy (G-VS)	ND, space, voltage[d]	$(256 \times 256) \times 1.6 \times 10^6$	400 GB



OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

Existing DR for NHOT - Matricization



- Works only when some of the dimensions are independent
- Matricizing NHOT is non-trivial

NTF and Piezoresponse Force Spectroscopy

- 3600 Vectorized Spatial Locations
- 128 Time Steps
- 16 different voltage steps

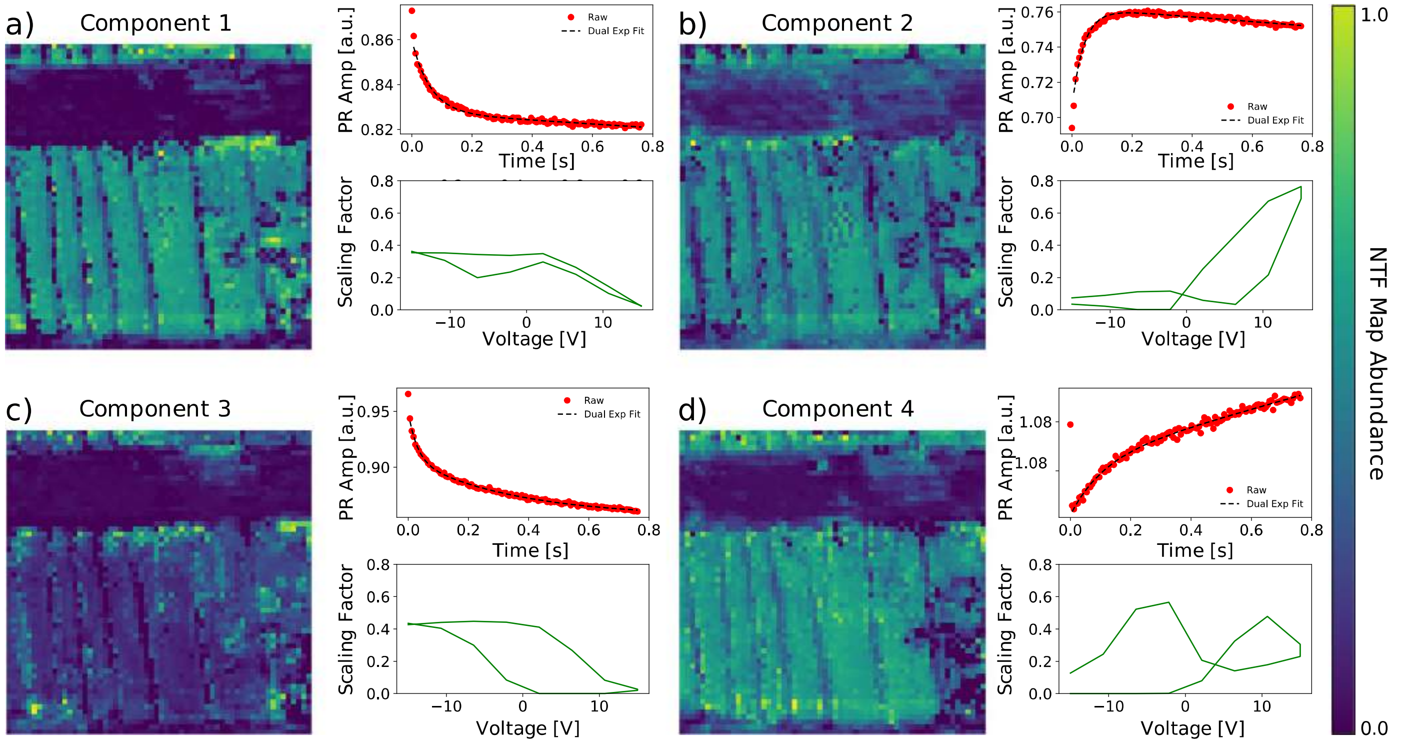
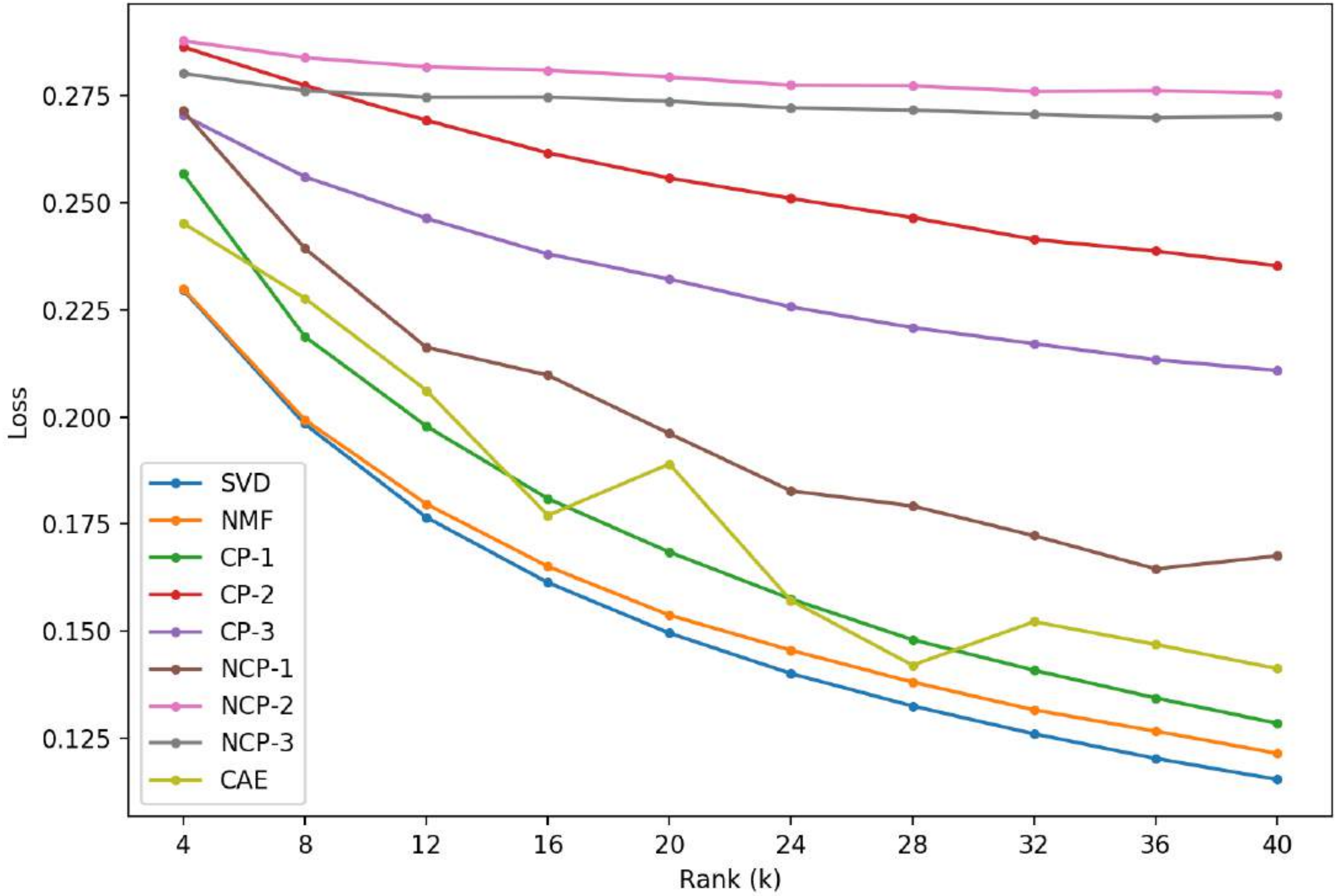


Fig. 4 NTF analysis on dynamic piezoresponse force microscopy data. Components 1–4 are shown in **a–d**, respectively, with corresponding relaxation behavior (time tensor factor, red) and voltage dependence (voltage tensor factor, green) plots. Large color maps correspond to normalized abundance maps for individual components.

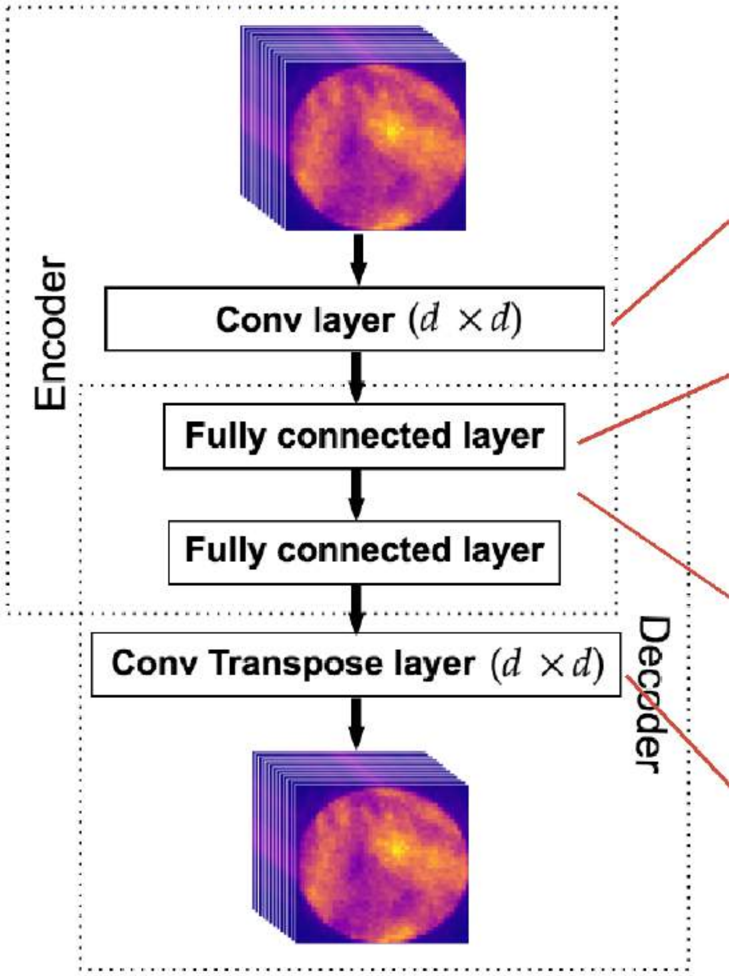
Kelley, K.P., Li, L., Ren, Y. *et al.* Tensor factorization for elucidating mechanisms of piezoresponse relaxation via dynamic Piezoresponse Force Spectroscopy. *npj Comput Mater* **6,** 113 (2020).

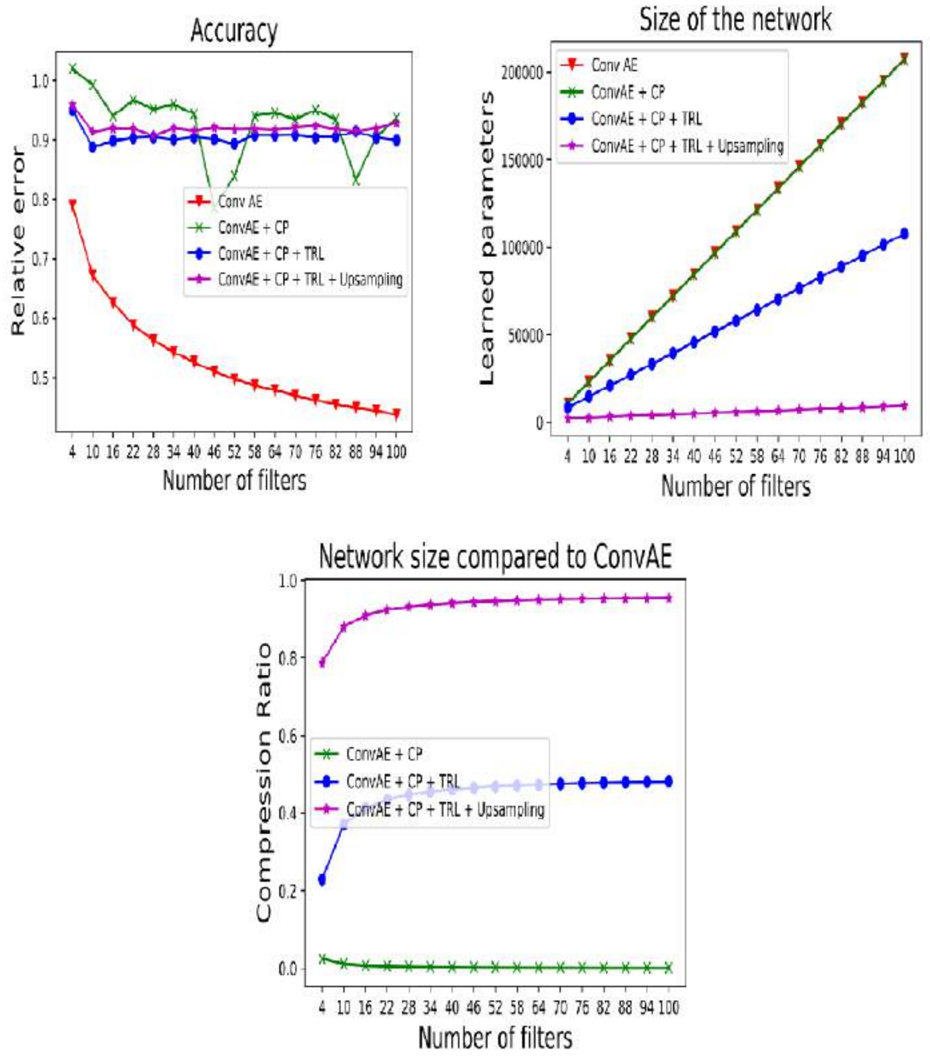
FLOPS vs Parameterization – Spatial Data



Pravi Devineni, Vagelis Papalexakis, Ramakrishnan Kannan

Convolutional Autoencoder





Thank You

NS&T ML-AI

Big Data **Machine Learning** **Artificial Intelligence**

Thank you