



Machine Learning and Data Science: Opportunities and Cautions in Science and Engineering

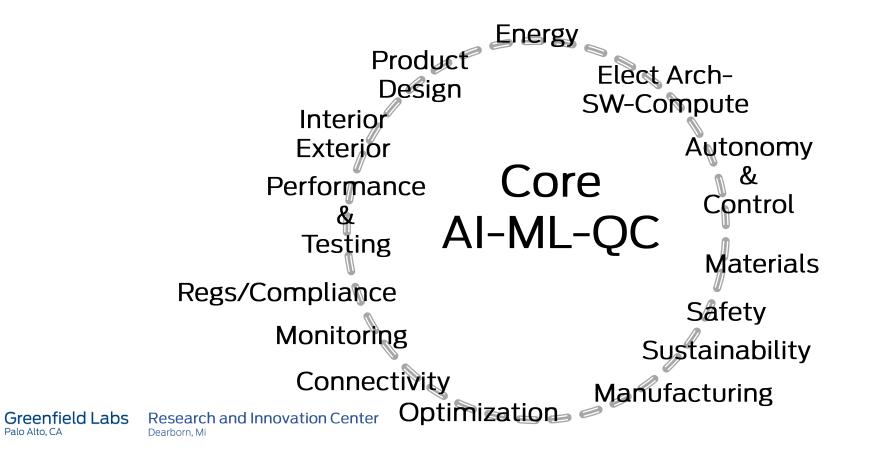
Discussions from initial efforts at Ford

Aug 10 2021

Devesh Upadhyay Core AI-ML Methods and Quantum Computing Ford Research

Focus

The intention of ML₄I is to <u>foster and illustrate</u> the <u>adoption of ML methods</u> for practical industrial outcomes. The forum will consist of a robust and open dialog between industry, research institutions, vendors, and academia to strengthen the technology transfer of ML methods to industrial needs.



Discussion today

We provide high lights of the problem domains, specific to the Automotive Industry, and discuss impacts and experiences of ML and data-sci .

- 1. Changing Landscape in Industry : Science, Engineering, Manufacturing
 - We discuss the Automotive Industry
 - We do not discuss Autonomous driving
- 2. Adoption of ML and Data Science in Engineering/Manufacturing □ Enablers , Pressures and Opportunities
- 3. Use cases ... some examples from industry (Ford) □ A mix of examples to show case the span of ML-Impact
- 4. Outlook, Opportunities , Challenges
 - Data
 - Robustness
 - □ Causality
 - Cautions



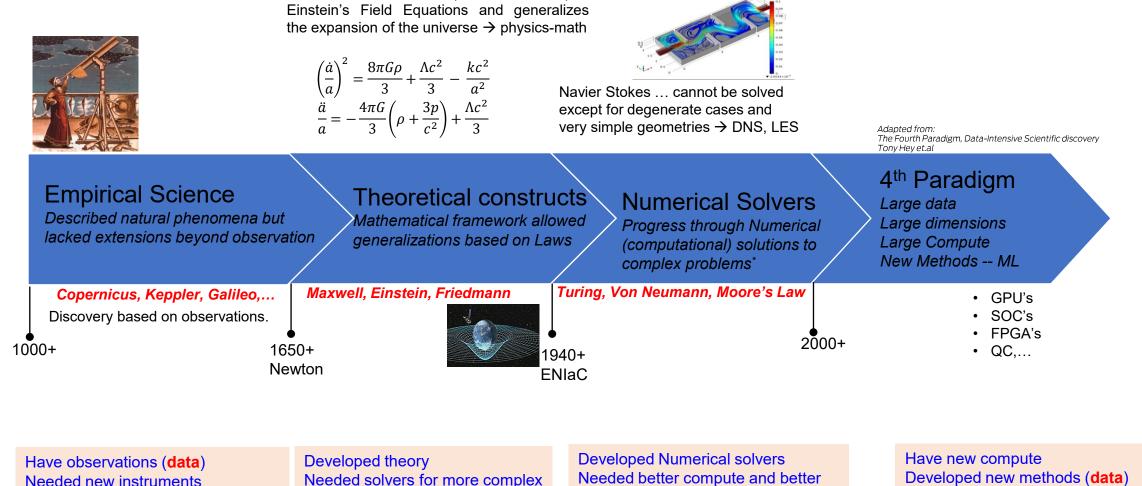
Changing Landscape in Science and Engineering

- We are in "The Fourth Paradigm"
- Science -- Engineering -- Manufacturing in industry
 - Old vs New
- Manufacturing Industry 4.0
- Labs of the Future
 - High throughput research
 - Looped Intelligence
 - Continuous testing and Calibration



Data-Models-Compute ... progression to the 4th paradigm

Friedmann's Cosmic equations built upon



numerical methods for speed Move to newer compute - QC

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problems

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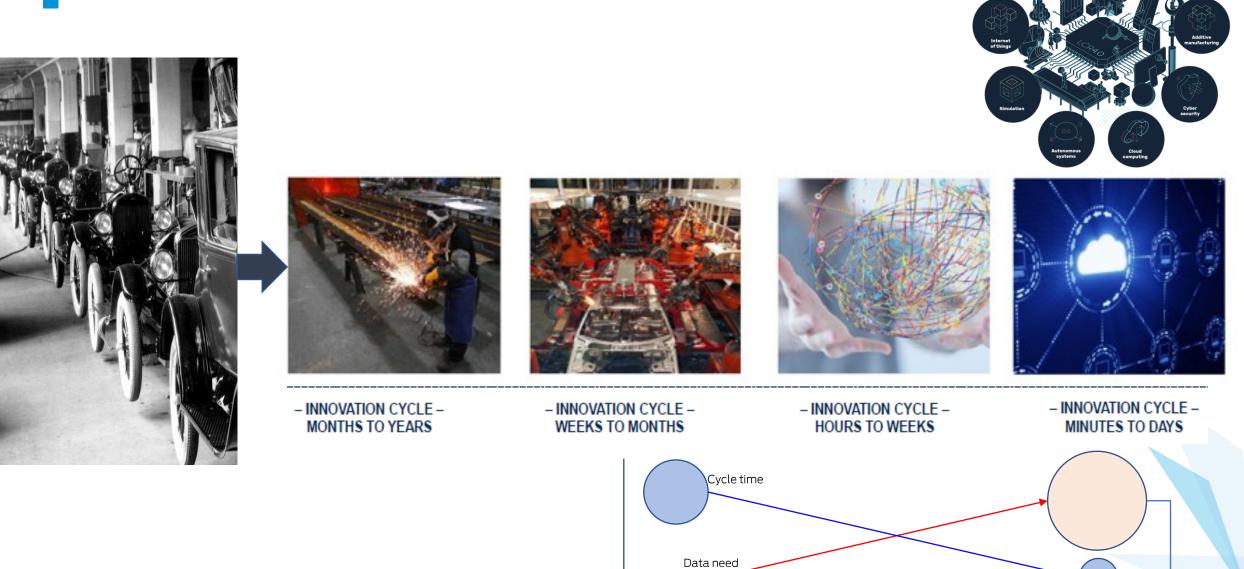
Needed theories for generalizations

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Science-Engineering & Manufacturing

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Improvements in cycle time drive data needs

Manufacturing: Industry 1.0 \rightarrow 4.0

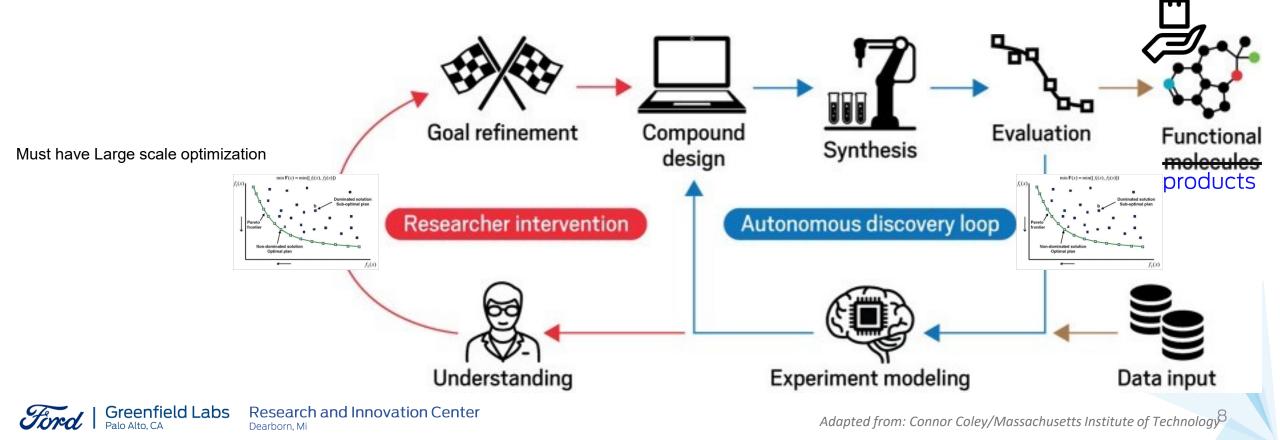
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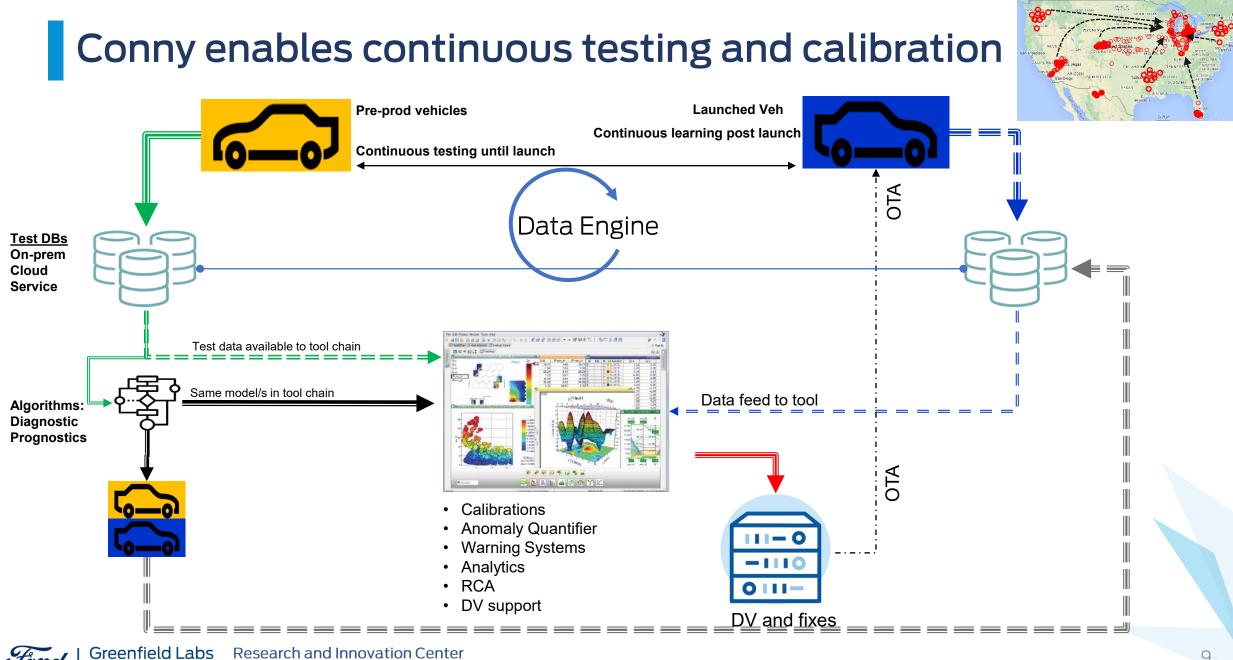
Ford

Accelerated discovery with Labs of the Future

LOOPED INTELLIGENCE

An autonomous chemistry laboratory runs experimental cycles intended to yield useful products molecules. In the cycle, artificial intelligence models the experiment and designs a product compound, robotic equipment runs the synthesis, and AI evaluates the output; researchers {and product designers} interpret the data and adjust experimental/design models or the goal definition as needed





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Adoption of ML and Data Science in Industry

3 key enablers for adoption

New sensing in vehicles and manufacturing

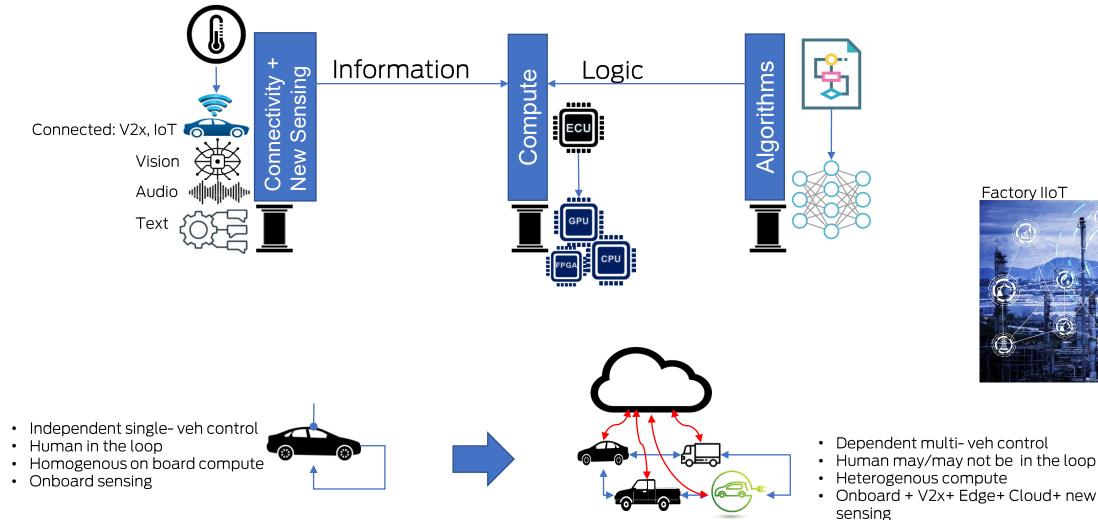
- Perception, IoT , IIoT (5G)
- Audio, Language

Demands/Pressures for adoption

- Need for high throughput research \rightarrow fast discovery
- Fresh look at high dimensional and/or complex problem domains
 - Need for high fidelity but fast surrogate models
- Automation -> Autonomy, Control
 - Vehicles
 - Mobility
 - Manufacturing
 - Robotics
 - :
- Asset Monitoring
 - Vehicles/Fleets
 - Manufacturing

Emerging technologies and a changing landscape

<u>**3- Pillars</u>**: 1. Connectivity + New Sensing, 2. Algorithms, 3. Compute</u>



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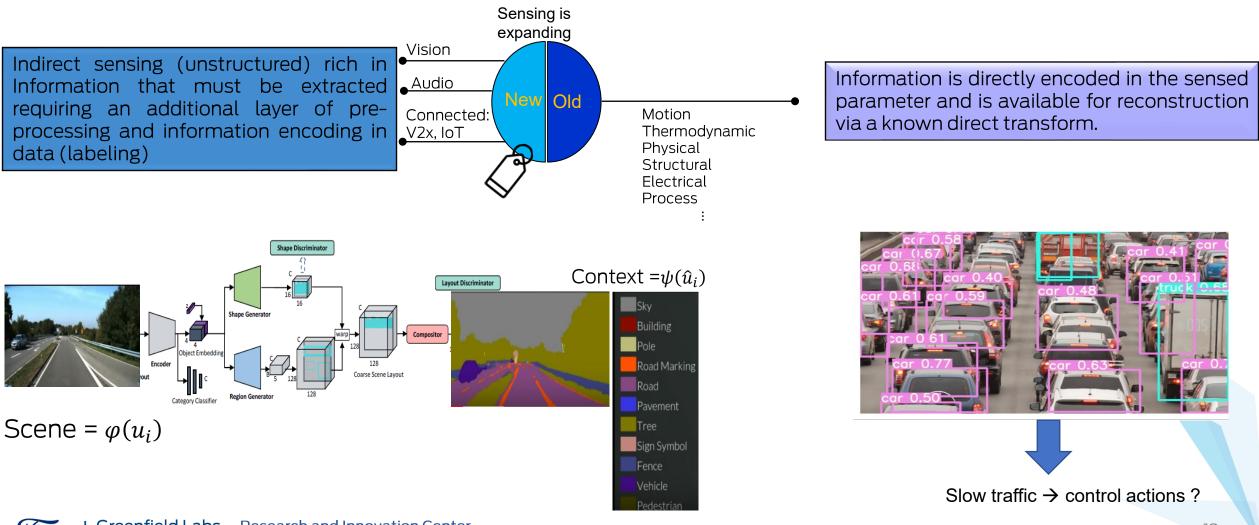
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Sensing \rightarrow new information sources are indirect sensing

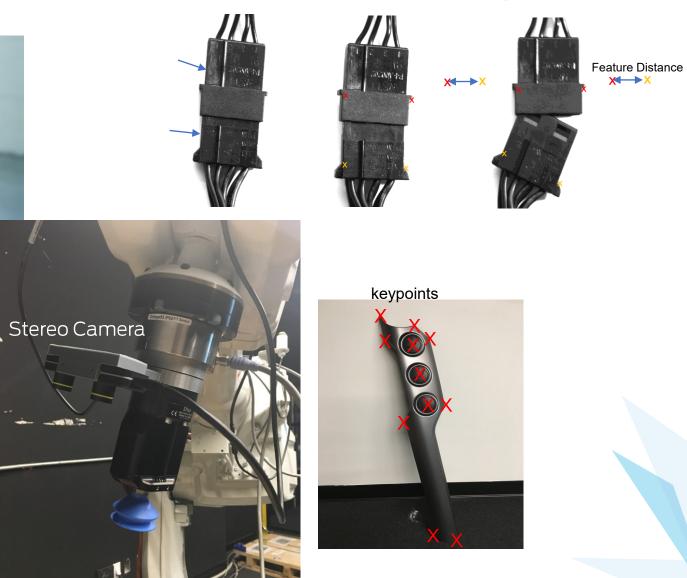


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Vision in Manufacturing



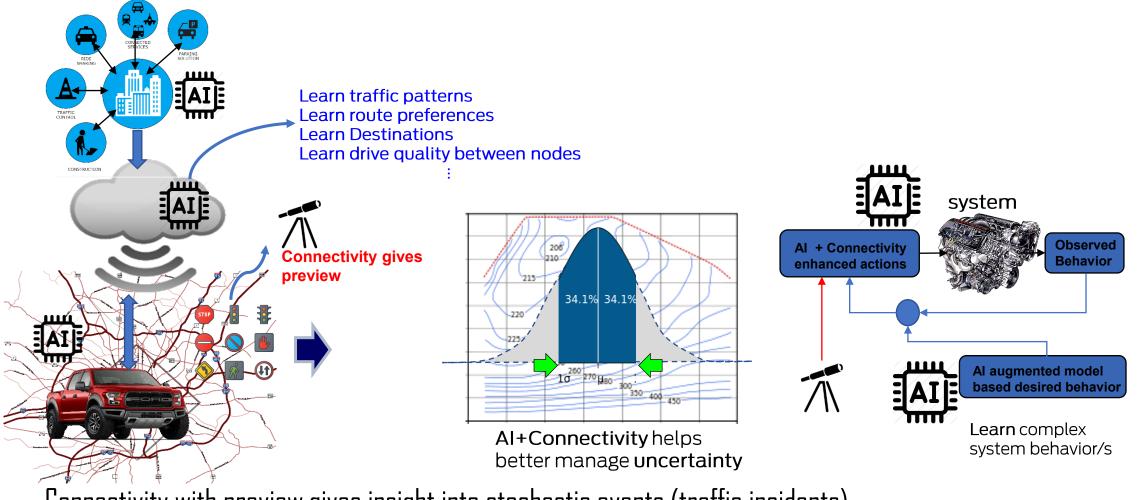
In situ error-proofing





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Connectivity and AI improve decisions under uncertainty through continuous Learning and exploiting preview



Connectivity with preview gives insight into stochastic events (traffic incidents). Combination of AI and Connectivity allows better management of uncertainty with improved Risk Reward trade-off.

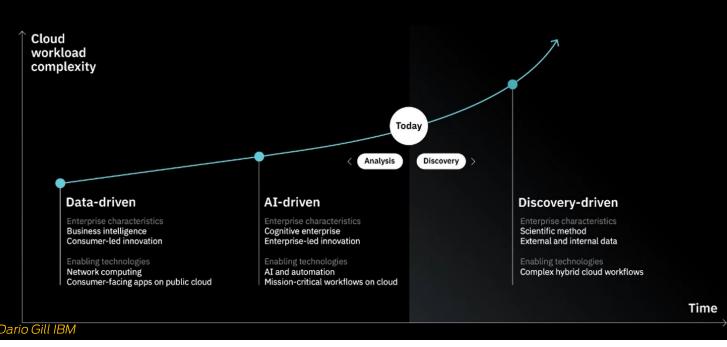
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Demands/Pressures

□ Fear of being left behind
 □ Industry must re-orient/adapt and choose carefully
 □ Industry must understand its data, adopt new tools, upskill and know where to apply ML.
 □ OTS solutions are typically NOT available for engineering problems → must create these
 □ Drives the demand for Engineers and Scientists to be proficient in ML
 □ There are many sellers of "false AI dreams" ... must carefully navigate between fact and fiction. Companies/Start-ups with multi-mil\$ valuations are selling "stuff" that used to be commonplace. Hence, in house expertise is needed to separate fact from fiction.

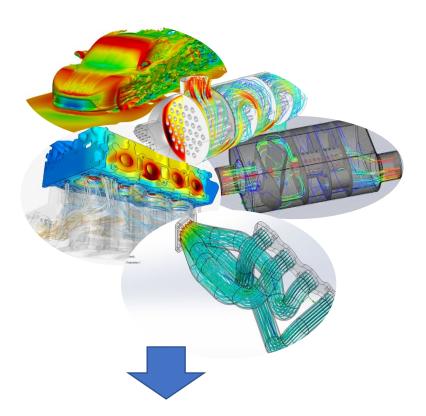
High throughput research: targeted discovery vs chance

Accelerated Discovery will provide a foundation for the Discovery-driven enterprise.





High dimensional, complex problem domains



Sim time can take "days" for a single run per case Curse of dimensionality \rightarrow formally ... computational cost increases with dimensionality of problem Ex. Finite difference discretization with *N* points per dimension and *d* dimensions requires compute over N^d points

3-D PDE with 1000 points per dimension \rightarrow 1000³ × 64 bits \approx 8GB RAM \rightarrow doable on a high-end laptop

4-D PDE with 1000 points per dimension \rightarrow 1000⁴ × 64 bits \approx 8TB Needs specialized nodes on HPC

5-D ... needs new compute

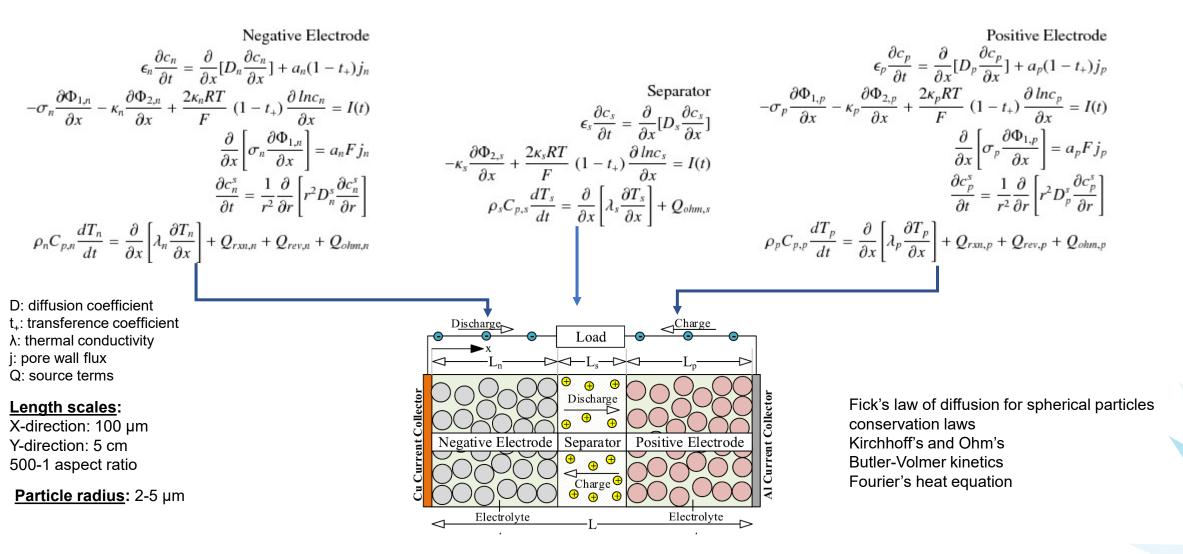
Images ... very high dimensional , MNIST 28x28 \rightarrow 784 dimensional input

Standard solvers \rightarrow Slow Simulations

PINNs → Less data, Interpretable, speed-up

Data Driven Models, Surrogates, ROMS, PINNS, Hybrids

High dimensional, complex problem domains: Li-lon batteries

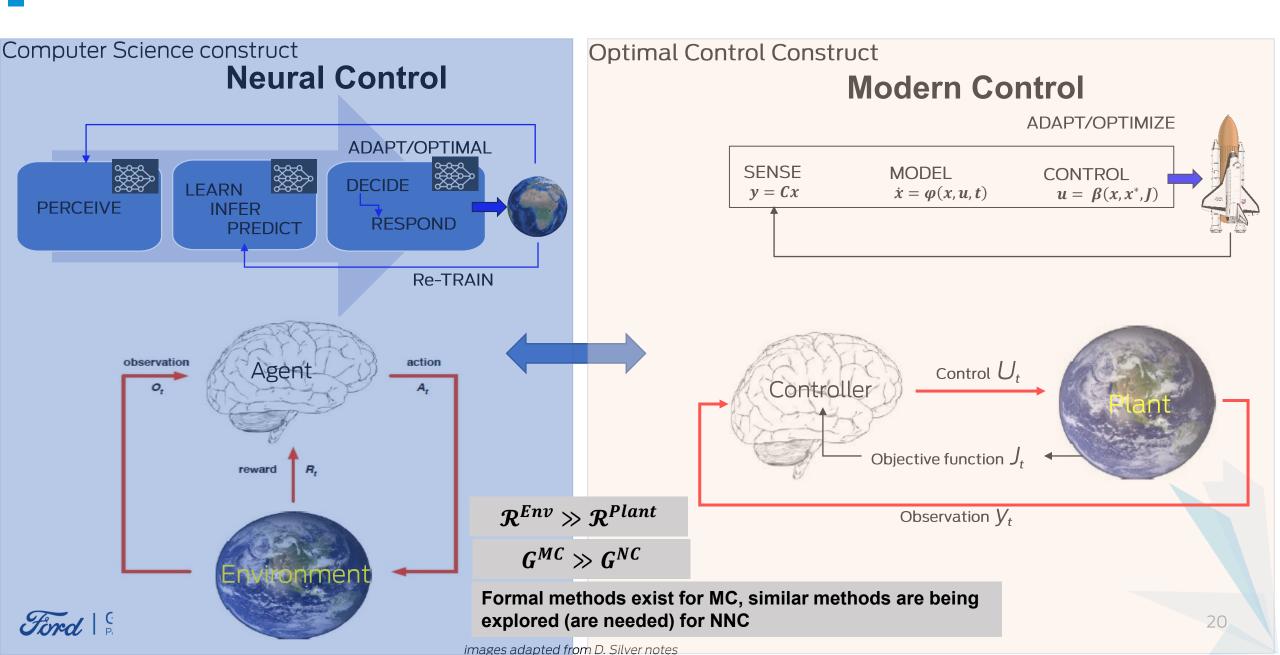


High dimensional, complex problem domains

- Just to note, there are many such problems across several domains in Science and Engineering.
- One fact that does stand out, and we will talk about this again, is the impact of these complexities on purely data driven re-constructions.
- For systems with high degrees of Nonlinearity, a data driven reconstruction of the system dynamic will typically require dense sampling across the domain of nonlinearity requiring *apriori* knowledge of the nonlinearities.
- Often such data will NOT be available, forcing a sparse representation and the use of techniques such as:
 - Compressed sensing
 - Bandwidth extension
 - and/or incremental learning from failures



Automation \rightarrow Control \rightarrow Autonomy



Autonomy, Mobility, Robotics



Home > News > Ford Invests In Argo AI, A New Artificial Intelligence Company, In Drive For Autonomous Vehicle Le

FORD INVESTS IN ARGO AI, A NEW ARTIFICIAL INTELLIGENCE COMPANY, IN DRIVE FOR AUTONOMOUS VEHICLE LEADERSHIP 000



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FIRST DIGIT ROBOTS TO FORD TO AGILITY ROBOTICS TO SELL ACCELERATE EXPLORATION OF COMMERCIAL VEHICLE CUSTOMER APPLICATIONS





NO BONES ABOUT IT: FORD EXPERIMENTS WITH FOUR-LEGGED ROBOTS, TO SCOUT FACTORIES, SAVING TIME, MONEY

Andia Kits

People Contacts Lincoln Bronce

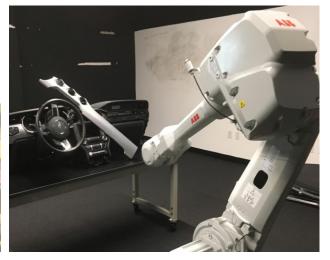
ries, Saving Time

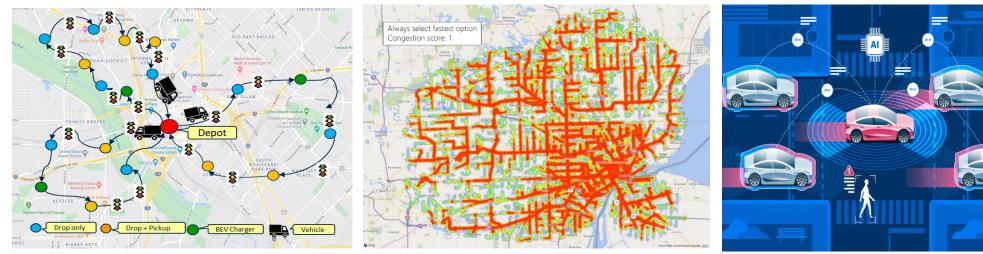
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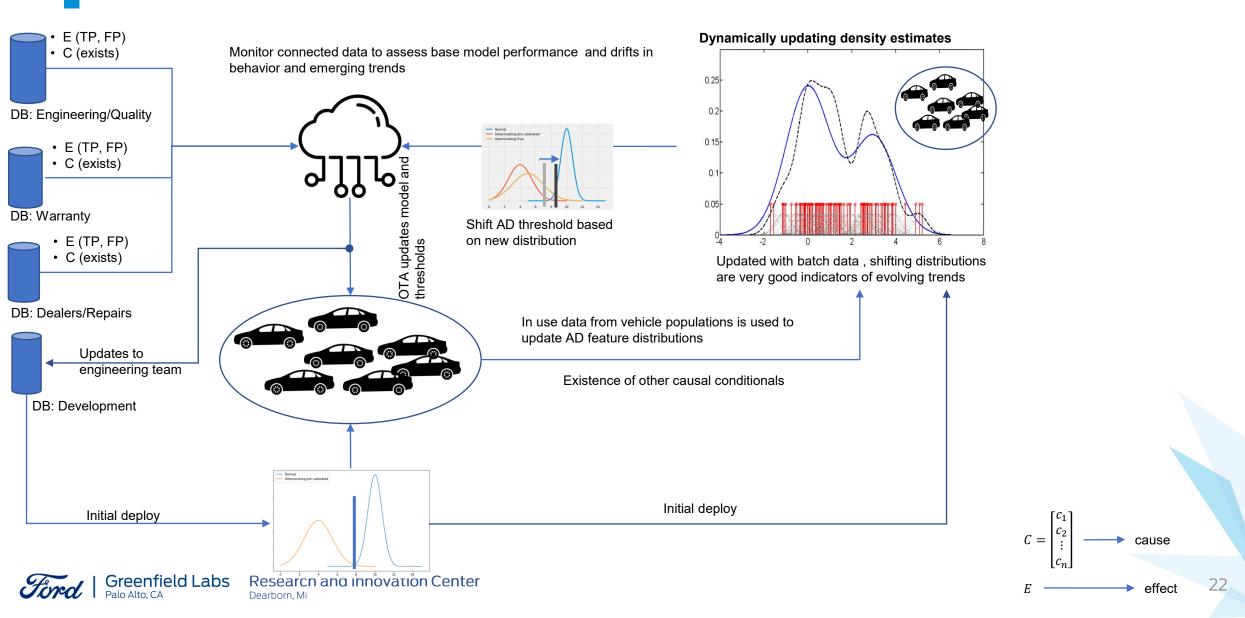








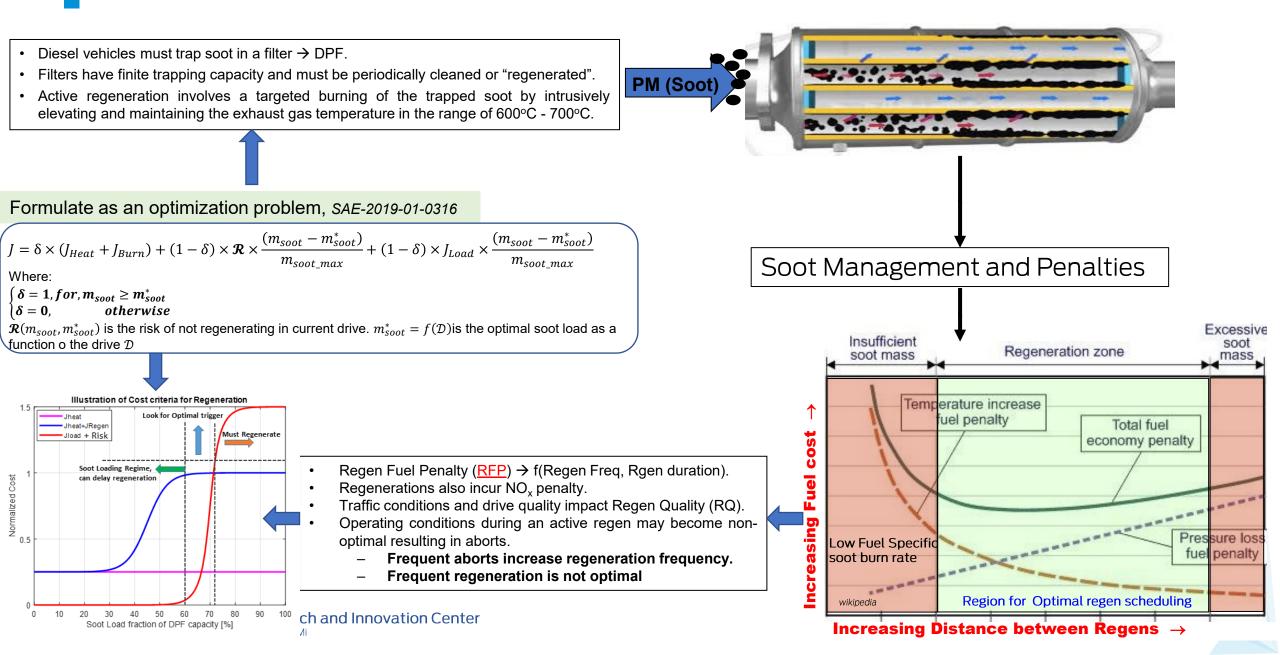
Monitoring: shifting to a distributed paradigm



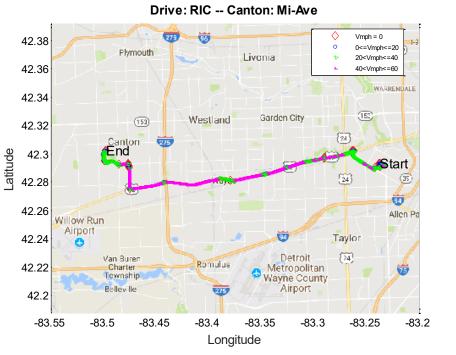
Case studies ... some examples

- Powertrain– Emissions Control
- Collision -- Vision systems and challenges
- Manufacturing process control, Robotics
- Material Science using images
- □ Charactering Sprays with Images
- □ Models (PINNS and Surrogates)
- □ Monitoring (OBD, vs AD&RUL)

Diesel Particulate filter – process and constraints



Naïve approach leads to short cycle regens

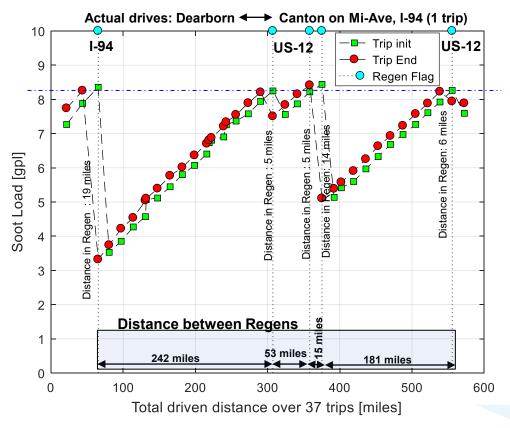


Soot Load (SL) at the start and end of each trip are shown $SL_{end} > SL_{start} \rightarrow loading cycle$ $SL_{end} \leq SL_{start} \rightarrow Regen cycle. (SL_{start} - SL_{end}) \rightarrow Soot load depleted$

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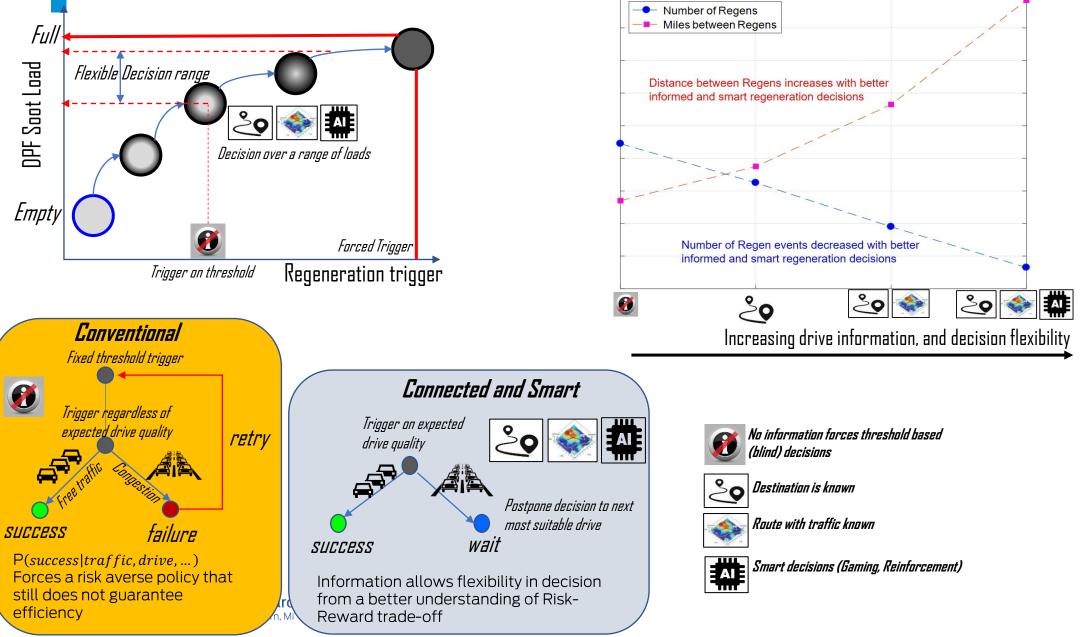
<u>Fixed SL- Threshold</u> based regen decisions can lead to short cycle regenerations resulting in increased regeneration frequency.

The probability of getting a deep regen (\geq 70%) is a strong function of the route and the likelihood of maintaining optimal regen conditions over the driven route.



Surrogates for fast sim and quantification

Drive information is an enabler toward more efficient regenerations



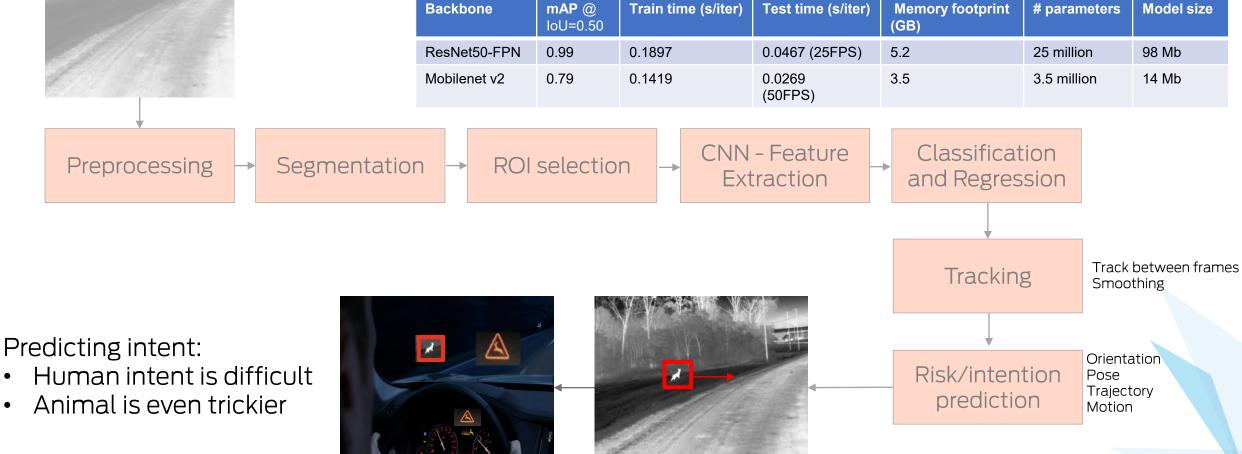
with A. Rahimpour

Vision based Collision avoidance with large animals.





Collisions with large animals such as deer and moose, etc. lead to about 200 human deaths and \$1.1 billion in property damage every year.

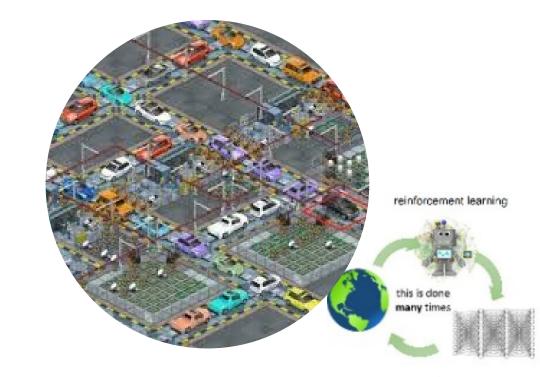




Manufacturing – Process control , Robotics, Error-proofing

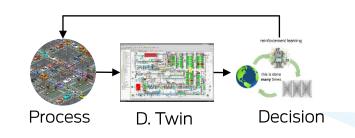
Assembly, Precision tasks, Inspection





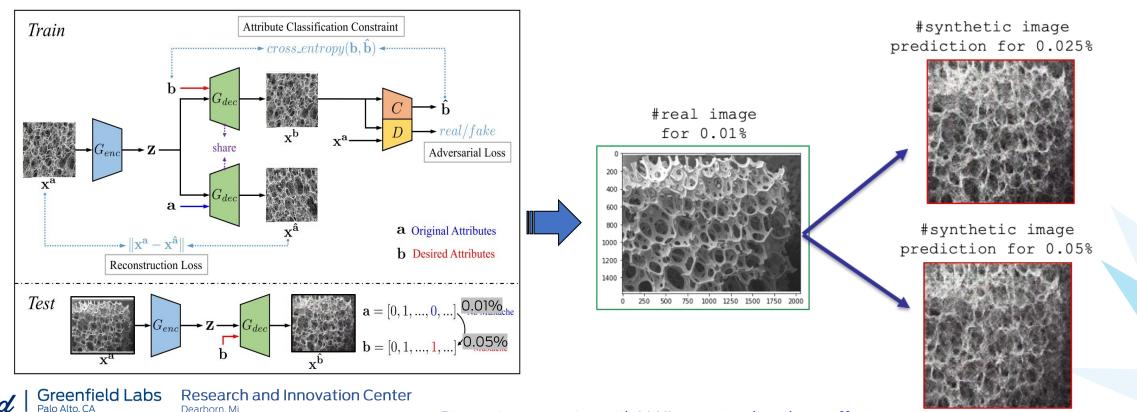
- Robots can assemble with repeated precision
- Grasping and manipulation tasks remain challenging
- Current end effectors are under-actuated systems
- Current robotics problems deal with parts designed for human assembly.

Assembly line process .. Pallett routing



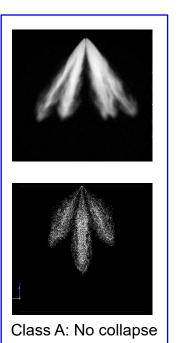
Material Science – using images

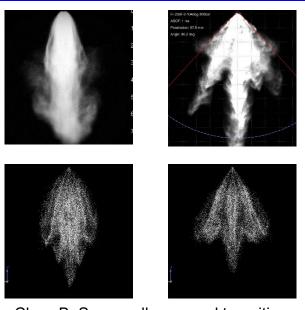
- An image editing generative adversarial network, AttGAN, was implemented to generate realistic synthetic SEM images showing subtle effect of the varied synthesis parameter of graphene additive %
- AttGAN avoids the large data requirement in GAN based design.
- Domain scientists can visualize and understand how changes in material attributes, synthesis/ processing conditions impact the sample microstructure features which in turn
 determine its properties and thus can further be optimized
- Needs fast imaging, SEM/FIB images, 2D vs 3D, defining structure level information is tricky
- Need to include physics based constraints



Discussions on going with LLNL on extending these efforts

Charactering Sprays with Images





Class B: Spray collapse, and transition

<u>Objective</u>: Injector nozzle design and Normally \rightarrow visual + CFD sims

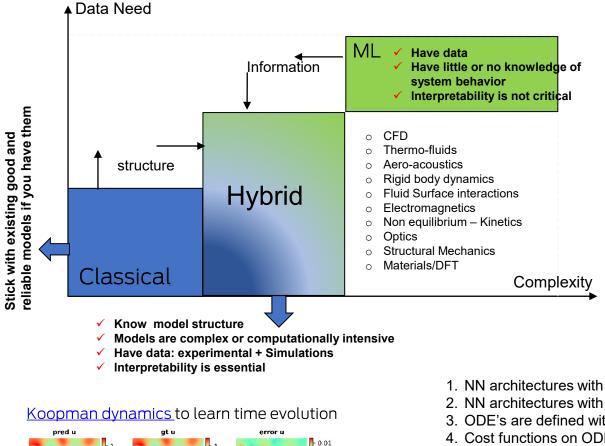
- Visual process too slow to keep up with fast imaging
- Prone to bias \rightarrow based on SME experience

<u>New → use CNN's</u>

- Major speed up in analysis
- Consistent and highly accurate and quantifiable results
- Transfer to other sprays/injectors
- Can further map to in-cylinder combustion performance
 measures and integrate into inverse design



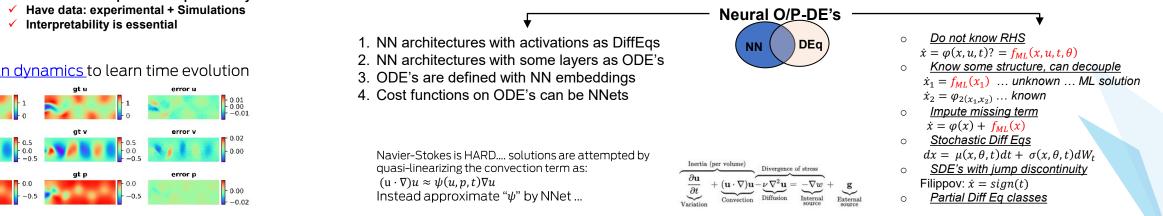
Models (PINNS and Surrogates)





- Universal approximation property of NNets →given enough layers a NN model can approximate any nonlinear function to within *ϵ* → good when nonlinearities are not known *apriori*.
 - $y_{ML}(x) = \sigma_3 \left(W_3 * \sigma_2 (W_2 * \sigma_1 (W_1 x)) \right) \rightarrow$ eg. a 3 layer network, NN's are function approximations: $\mathcal{R}^n \rightarrow \mathcal{R}^m$
- □ Differential equations are compact ways of specifying arbitrary nonlinear transforms by mathematically encoding prior structural assumptions → good when nonlinearities are known *apriori* → $\dot{x} = \varphi(x, u, t)$
- Both are differentiable.

Include domain knowledge in ML : Scientific ML



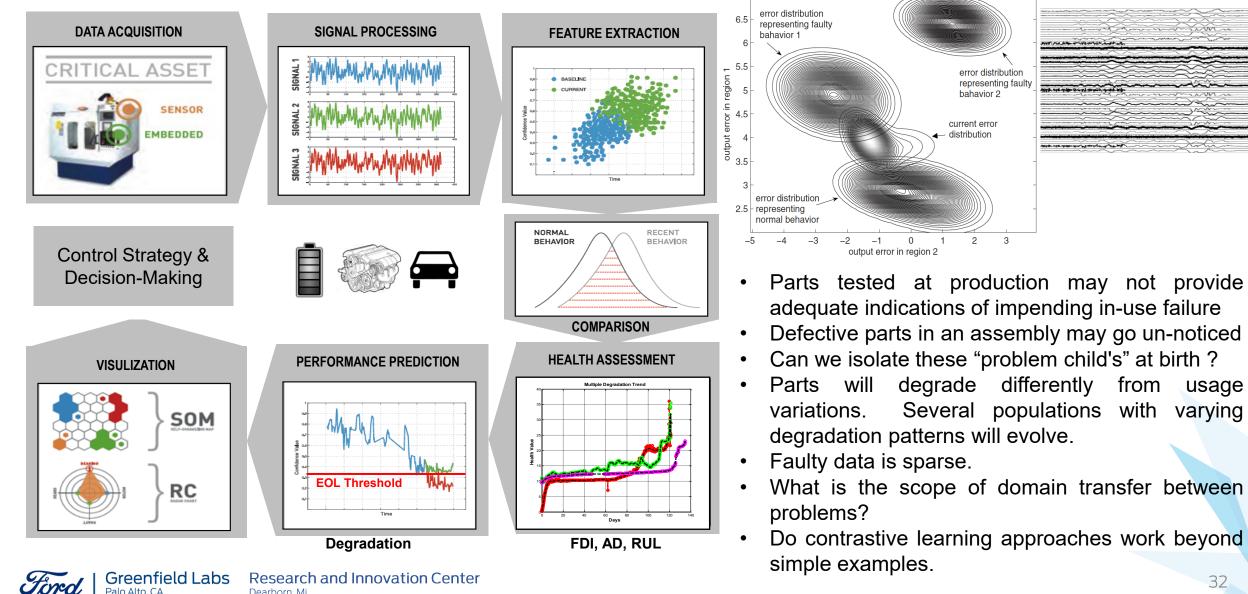
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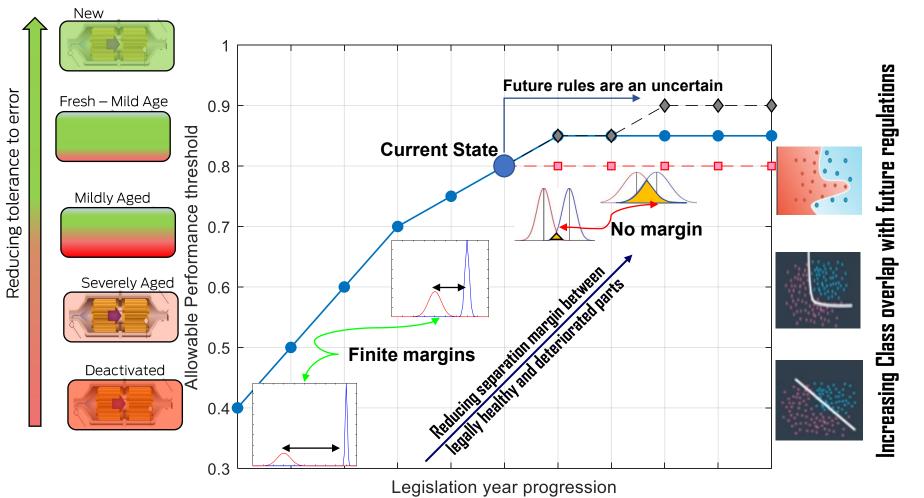
NeuralPDE: Automating Physics-Informed Neural Networks (PINNs) with Error Approximations, to appear in arXiv

Anomaly Detection: Use ML for multivariate problems



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On-Board Diagnostics (OBD) with future rule making



Isolating failed parts is easy (most of ML based AD today), isolating functional parts with marginal deterioration and multiple dependencies ... not so easy

Outlook, Opportunities and Challenges

Data

- How much data and how to get it optimally
- The data trap: "too much data with very little information"

Robustness

- Data drift/bias/coverage
- Models drift/bias
- Safety– in RL (exploration), neural controllers, controllers with perception

Causality

- Generalization /Explainability
- UQ (of Data and Model)
- Embedding physics \rightarrow PINNs, Hybrid methods

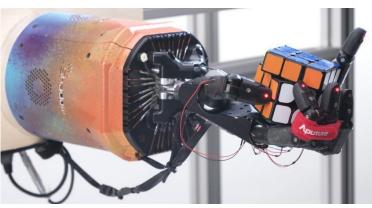
Cautions

- Regulations , Safety and Guidance
- Deployment, CI-CD is now CI-CD-CM
- Fact Vs Fiction
- The "AI-Hammer" effect



Data: How much ? Costs? Manage, Label, Drift

OpenAI disbands its robotics research team VB July 2021



OpenAl has disbanded its robotics team after years of research into machines that can learn to perform tasks like <u>solving a Rubik's Cube</u>. Company cofounder Wojciech Zaremba quietly revealed on a <u>podcast</u> hosted by startup Weights & Biases that OpenAl has shifted its focus to other domains, where data is more readily available.

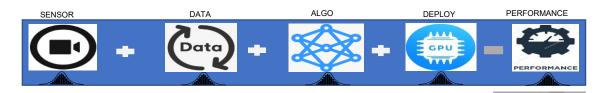
"So it turns out that we <u>can make a gigantic progress whenever we have access to data</u>".

Slightly misleading its not just data but LARGE DATA

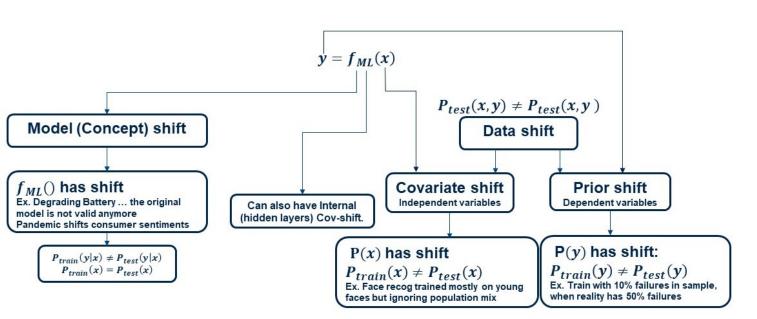
- Is data a good substitute for Physics ? Ignoring physics implies data must re-learn the system → Increased data burden and all associated risks/errors.
- Extracting full domain representation from data alone requires a data set with very dense representation → which usually translates to aggregation of a lot of data with sparse representations
- Data needing labeling (indirect sensing) are prone to noisy labels and impact learning !
- Purely data driven models need to learn continuously (hence need new data) until full coverage of domain, but by then system/domain may have drifted !
 - Tesla trains FSD with 1.5PB \rightarrow building their own cluster 5760 A100 GPUs
- Need an "intelligent" Data and Learning policy.

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Robustness (of ML models)



- Industrial and Engineering systems need guarantees and must be explainable!
 - Design, Safety, Performance, ...
- ML methods, in general, lack formal approaches to understanding robustness, reliability, stability etc, but this may be changing !
- ML models rely on data, both data and models will have biases and can also drift → requires robustness checks at build as well as constant
 monitoring post deployment. → Past performance is no guarantee of future results !!
- Corner cases (more frequent than edge) vs Edge cases (did not think of these but Pr () >0 = unknown unknowns).
 - One may inadvertently transition into regions where Pr(Edge) increases!
- ASIL-B → < 1 Failure in 10⁷ hours of driving. At ~ 60mph that is 6x10⁸ miles of driving = 0.6B miles of driving. At 150K Miles vehicle useful life this is equivalent to data from 4000 cars driven to full useful life !!
- Currently Robustness implies massive amounts of testing, Simulation + Real life \rightarrow different impacts depending on data class.

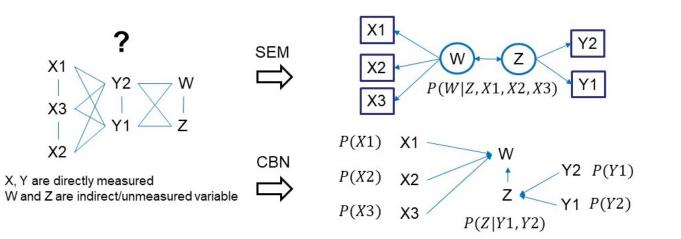




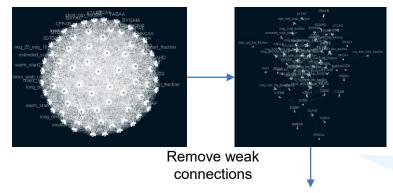
Corner or edge?



- Recently there has been growing interest in the CS-ML community to address causality (Yoshua Bengio, Hinton, LeCunn), Others, Pearl Marcus, etc have been asking for this.
- Understanding causality is critical in engineering/manufacturing systems
 - What is the root cause ? Formally (statistically) ... determine if a change in a given "treatment" leads to a change in some outcome → sensitivity analysis (engineering speak)
 - Humans can only manage short chain credit assignments, for multivariate influences ... need compute
 - Extracting causality from pixel space is more difficult
- Discover causal relations by analyzing statistical properties of purely observational data
 - Expert knowledge: collection of facts and heuristics about the system
 - Granger causality: causality in time series data
 - Structural Equation Modeling (SEM): what factors determined the variable value
 - Casual Bayesian Network (CBN): what the probability of the variable changes when changing factors
 - Causal calculus ('Pearl')
- Causality in the action space recovering from changes
 - Distributions (system representations) will change due to environmental pressures and/or direct intervention
 - Good causal models allow Causal induction from interventions .. Can we estimate the intervention



Extract the largest subgraph with target attribute



Classifv

Cautions

• Regulations , Safety and Guidance

- Most ML models will not satisfy current regulatory obligations, typically requiring > 99.99 accuracies.
- Currently there is no mechanism to re-certify models that re-train on the fly.
- Blame assignment remains an open question
- Are simulators a good substitute, for real world testing ? This drives the need for "certifiably correct simulators"
- Synthetic data and Photo real vs PBR (Light Structure interactions)
- Deployment, CI/CD is now CI/CD-CM
 - ML SW when deployed requires continuous monitoring (CM) given that models and data will drift as we discussed

Fact and Fiction

- Buyers beware ! This drives the need for in-house expertise.
- There is an explosion of jargon that can be unnerving and quite tricky to navigate.
- Beware of "Dashboards", front ends can be dangerous.
- The "AI-Hammer" effect
 - Everything looks like a nail, and it sells (surprisingly)
 - OTS, pretrained networks are becoming commoditized, and there is a tendency to just train and re-train.
 - Strict quality control of ML models, in an industrial setting, is still evolving

Thank you for your time



- This presentation had contributions from several people on the Core AI-ML-QC team in Ford Research
 - Alireza Rahimpour, Alemayehu Admasu, Huanyi Shui, Harshal Maske, Hongjiang Li, Kaushik Balakrishnan, Mike Hopka, Patrick Blanchard (and his team) and the rest of the Core AI-ML-QC team.
- Guidance and support from: John Schneider (Director ESCAIT), Dimitar Filev (Tech. Fellow)
- We also included some results on PINNs from an ongoing project with MIT (Prof. Alan Edelman, Chris Rackuackas, et.al



