A few words about me: disruptions, Machine Learning, real-time, mentoring, teaching & education

(2014) PhD in Physics, University of Padova, Italy
(2015) Data Scientist, UniCredit, Milan, Italy
(2016) Postdoctoral Associate, MIT PSFC
(2019) Research Scientist, MIT PSFC
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AI & ML in Fusion

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Introduction to Fusion Energy and Plasma Physics Course, PPPL and remote, June 15th, 2023



Outline

- 1. Fusion stuff and disruptions!
- 2. The Universality theorem and brief ML taxonomy
- 3. Explainable and adaptive ML models applications in Fusion
- 4. Current challenges and opportunities for future research
- 5. Conclusions

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Fusion research is tackling transformational technologies to provide alternative, carbon-free electricity generation





$D+T \rightarrow \alpha$ (3.5 MeV) + n(14.1 MeV)

Lab research conducted via:

Heating and confinement of a plasma of hydrogen isotopes via magnetic fields → magnetic confinement

Moser's and Paul's lecture

 Heating and compressing via lasers a fuel target of hydrogen isotopes → inertial confinement

Malko's and Kritcher's lecture

IFE

Au or DU

hohlraum

Let's take a closer look at MFE plasmas.



Capsule fill tube

time of the second second

Fusion Plasmas: nonlinear phenomena really hot or really fast, hard to diagnose, lots theory & exp data, not so easy to bridge



Challenges in thermonuclear fusion simulation: "The tyranny of scales"

Fusion plasma dynamics spanning wide range of spatial and temporal scales

Not so easy to develop first principle solutions!



Many operating experimental devices for magnetically confined fusion research, more planned!



IAEA Fusion Device Information System https://www.iter.org/of-interest/944 Huge amount of experimental and simulation data available enabling **Machine Learning applications:**

- optimization of experimental design
- real-time monitoring of proximity to instability
- trajectory planning optimization
- fast surrogates to accelerate simulations

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proximity to instability

trajectory planning optimization

fast surrogates to accelerate simulations

Active monitoring and prediction of soft/hard limits necessary to inform transition across operational boundaries



Adapted from J. Barr IAEA TM PDM 2020

Interpretable/explainable data-driven models provide general proximity to unstable operational space

Plasma pushed close to operational limits often leads to instabilities onset or control faults: disruptions!



Major disruption \rightarrow final loss of control evolving on timescales of milliseconds:

- Fast drop I_p leads to loss of confining poloidal field.
- Fast I_p transient causes large induced voltages, currents, forces.
- Rapid thermal losses cause surface damage.

Plasma pushed close to operational limits often leads to instabilities onset or control faults: disruptions!



Visible camera view of RE beam hitting Alcator C-Mod first wall. Courtesy R.A. Tinguely

JET runaway electrons damage. https://www.iter.org/newsline/-/2234

How to take care of disruptions:

- Accept the damage and live with it.
- Mitigate the damage by injecting massive gas or shattered pellets.
- Avoid altogether by detecting <u>precursors</u> & steer plasma away from disruptive boundary.

Precursor's growth prediction and detection extremely important...



ITER Physics Expert Group on Disruptions, Plasma Control, and MHD (1999) Nucl. Fusion 39 2251

...but not an easy task! Statistical studies show complex chains of events:

possible disruptive chains of events



- Similar **statistical studies** not always available across different tokamaks.
- Need timely identification of precursors to allow the plasma control system (PCS) to take proper action.

Wealth of experimental data from different tokamaks enables Machine Learning applications.

Statistics of the sequence of events for ~10yrs of unintentional disruptions at JET: width of the connecting arrows is the frequency of event occurrence.

De Vries et al. NF 51 (2011) 053018 "Survey of disruption causes at JET"

Explainable ML models for disruption prediction useful resources to identify stability boundaries in real-time

 DIII-D/EAST: the Disruption Prediction via Random Forest algorithm (DPRF) applied to compute the probability of an impending disruption, while interpreting its drivers in real-time.



C. Rea et al, 2021 IAEA EX/P1–25, J. Barr et al, Nucl. Fusion 61 (2021) 126019

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Sometimes there's confusion about terminology, too many buzzwords!



To **mimic human behavior** and functions such as **learning** and **problem solving**.

Al subset using **statistical methods** to enable **learn-from-experience** paradigm.

ML subset with broader **generalization** capabilities – **neural networks**.





From biological to artificial neurons: the computational graph



From biological to artificial neurons: the computational graph



The Universality Theorem: for <u>any arbitrary f(x)</u>, there is <u>always</u> an artificial neural network that can <u>approximate</u> it

$$y \approx f(x) = f^{(4)}(f^{(3)}(f^{(2)}(f^{(1)}(x))))$$



Caveats:

- Increasing the depth can improve the <u>approximation</u>. $|y - f(\mathbf{x})| < \varepsilon$
- Activation must be <u>continuous</u>.

Neural networks provide nonlinear mapping from inputs to outputs, or a way to represent your data through function approximation and estimation.

Deep neural network example, adapted from B. Spears et al PoP 2018

Statistical inference to learn representations from available data



Statistical inference to learn representations from available data



Introducing the black box: the issue with high-stakes decision making ...



Black box as either

- function **too complicated** for human to comprehend or
- function that is **proprietary**

C. Rudin, Nat Mach Intell 1, 206–215 (2019)

Implications:

- lack of transparency and accountability,
- troubleshooting challenges.

High-stakes decision making:

- healthcare,
- criminal justice,
- child welfare screening,
- self-driving cars,

• ...

High-stakes decision making and the parallelism with the fusion context



D. Humphreys et al, 2020 Advancing Fusion with Machine Learning Research Needs Workshop Report, J. Fusion Energy 39 123–55

23 Intro and fundamentals



Fusion energy systems:

Any ML-based decision needs to be **trusted** and **justified**, or *licensed* \rightarrow high-stake decisions!

Science discovery → Reconciliation with physical understanding, key ingredient to advance fusion research.



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https://xkcd.com/2541/

Common perception of accuracy vs interpretability trade-off



Model Interpretability

25 Explainability vs interpretability

More interpretable and simpler models can be as accurate as black boxes



Model Interpretability

26 Explainability vs interpretability

More interpretable and simpler models can be as accurate as black boxes



Model Interpretability

No unique "interpretability" definition:

- It's algorithm dependent e.g., possibility to inspect reasons.
- It's domain dependent e.g. sparsity not good for natural image classification.

More interpretable and simpler models can be as accurate as black boxes



Model Interpretability

No unique "interpretability" definition:

- It's algorithm dependent e.g., possibility to inspect reasons.
- It's domain dependent e.g. sparsity not good for natural image classification.

What about accuracy definition?

 Typically well-defined – e.g., counting statistics of misclassifications, root mean squared error,

. . .



ML systems' prediction accuracy measured on new test data ...

Simplified supervised ML classification workflow:

2D example (blue vs red)

Adapted from A. Pau et al, Nuclear Fusion, 59(10):106017, 2019



... by counting how many times the trained classifier is right or wrong!



True Positive Rate: # correct positive classifications

total # of **positive** samples

False Positive Rate: # wrong positive classifications

total # **negative** samples

ML models of varying complexity can have comparable performances – a disruption prediction example



Fusion

• Rashomon Effect:

a multitude of models with approximately the minimum error rate exists, for many problems¹ (also in Fusion!).

As long as a large Rashomon set exists, it is likely that some are interpretable^{2,3}, maybe hard to develop.

¹L. Breiman et al, 2001 Statistical Science 16 199–231 ²C. Rudin et al., 2022 Stat. Surv. 16 1–85 ³Semenova et al, 2022 ACM Conference on Fairness, Accountability, and Transparency (FAccT'22) arXiv:1908.01755

Adapted from J. Kates-Harbeck et al., Nature 568, 526-531 (2019)

ML models of varying complexity with comparable performances





https://en.wikipedia.org/wiki/Rashomon

<u>Fun fact</u>: Rashomon term inspired by 1950 Kurosawa's movie!

Rashomon Effect:

a multitude of models with approximately the minimum error rate exists, for many problems¹ (also in Fusion!).

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¹L. Breiman et al, 2001 Statistical Science 16 199–231
²C. Rudin et al., 2022 Stat. Surv. 16 1–85
³Semenova et al, 2022 ACM Conference on Fairness, Accountability, and Transparency (FAccT'22) arXiv:1908.01755

Models interpretable by design vs black boxes that can be "explained"



33 Explainability vs interpretability

Models interpretable by design vs black boxes that can be "explained"



34 Explainability vs interpretability

Dimensionality reduction (DR) enables inspection of dataset structure



C. Rudin et al., 2022 Stat. Surv. 16 1–85

- Latent space (no physical units) allows 2D visualization of **similar data points** in high-dimensional feature space. Coloring done a-posteriori!
 - All DR methods allow some form of data inspection and understanding.
- 35 Explainability vs interpretability

Clustering algorithms enable discovery of data patterns



J.X. Zhu, C. Rea et al, 2021 Nucl. Fusion 61 114005

36 Explainability vs interpretability
Explainable ML predictions for real-time proximity to instability – a Random Forest example



Advantages:

Adapted from: "Random Forest Regression," levelup.gitconnected.com

- Identification of stability boundaries in real-time.
- Local explainability metrics leveraged inside controllers to modify plasma trajectory in real-time.

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Identification of safe operating region through fast ML enables trajectory planning



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https://xkcd.com/1781/

Data drives fusion experiments' design, simulation, analysis, control and optimization – enabling science discovery



Adapted from D. Humphreys et al. "Advancing Fusion With Machine Learning" DOE Workshop (2020)



D. Humphreys et al. "Advancing Fusion With Machine Learning" DOE Workshop (2020)

Pilot plants and next gen devices need robust models featuring

- interpretability/explainability
- well-defined validity and extrapolability boundaries

• ..

ML requires large datasets with target events labeled



Labeling events often requires manual inspection of multiple signals: semi-supervised ML accelerates event labeling



Partially Labeled Event Data



- Common signals from many shots
- A fraction (at least 1 shot) has labeled event occurrence

Semi-Supervised Learner

- Use unlabeled data distribution to find other events
- Output times when event likely occurred

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Semi-supervised label spreading algorithm to automate detection of physics events



Can be applied to accelerate the construction of events databases

- Iteratively choose initially labeled shot from set of marginal detections
- Prediction quality on unlabeled shots improves consistently
 - Detected events in $\sim 85\%$ of hundreds of shots after manually analyzing just $\sim 1\%$



Data augmentation to learn disruptive dynamics (I)



- DL models are data-greedy: need comprehensive training database to achieve satisfying and reliable results.
- Robust augmentation of the training database using
 state space Student-T surrogate models.

Rath, (...), Rea et al, "Data augmentation for disruption prediction via robust surrogate models" J. Plasma Phys. (2022), vol. 88, 895880502

Data augmentation to learn disruptive dynamics (II)



- random time warping 5 times in parallel,
- random crop subsequences with length 300,
- random quantize to 10-, 20-, or 30- level sets,
- with 80% probability , random drift the signal up to 10% 50%,
- with 50% probability, reverse the sequence.



Predict "time-to-disruption" risk using classification probability



Any classification probability (P_D) cast between [0,1] can be used to:

- Predict the future probability of plasma survival S(t+Δt | t) [1] or
- Model the instantaneous hazard [2,3] h=d lnS/dt to be used as probability generator.

Hazard function modeling connects dynamical systems and risk-aware control design by probability generation.

C-Mod data used as proof of concept to combine DPRF (or <u>any classifier</u>) disruptivity with survival analysis.

RA Tinguely et al 2019 PPCF 61
 KEJ Olofsson et al 2018 PPCF 60
 KEJ Olofsson et al 2018 FED 146
 Continued work by Z. Keith, C. Rea (MIT)

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Hybrid Deep Learning predictor for cross-machine disruption prediction using time series data



Adaptive strategies designed to optimize predictions across different fusion devices

- Adapt current state-of-the-art ML predictors to different operational regimes across devices (DIII-D/EAST).
- Implications for next-gen, yet-to-be-built devices!
- Adaptive strategies:
 - ad-hoc design of training sets to match target domain by fully exploiting existing data¹,
 - **retrain predictors** after performance degradation².

Adapted from ¹J.X. Zhu et al, NF (2021) 114005 ²J. Vega et al., *Nat. Phys.* 18, 741–750 (2022)

Task: predict DIII-D HP FPR = 0.10.9 0.8 Training sets: DIII-D LP 0.3 DILL-D DIII-D LP + EAST HP 0.2 Other combinations 0.1 0 0 0.02 0.18 0.04 0.06 0.12 0.14 0.16 0.2 0.08

False positive rate

Domain adaptation

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Fusion

Existing current challenges in ML-applied research 😟 but also (!) opportunities for future scientists 👰

- trust in performance metrics → missing benchmarks
- trust in predictive output and learning → model interpretation and explanation accuracy
- prediction of out of distribution samples \rightarrow **domain shifts**, **data shifts**
- integration with legacy architectures \rightarrow real-time vs offline implementations
- lack of labeled data or of reliable (and automated) metadata extraction
- uncertainty quantification
- open and FAIR (!) access to data and models



M. Wilkinson, *et al.* The FAIR Guiding Principles for scientific data management and stewardship. *Sci Data* **3**, 160018 (2016)



UNESCO Recommendation on Open Science

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DOE and International Agencies strongly support ML research to accelerate Fusion progress

- 2019 DOE-sponsored workshop critical PROs identified
- \rightarrow
- DOE Public Reusable Research Data (PuRE) initiative

https://science.osti.gov/Initiatives/PuRe-Data

• IAEA Coordinated Research Project addressing cross-cutting issues

Workshop on Advancing Fusion with Machine Learning Priority Research Opportunities (PROs)

Accelerating Science	Enabling Fusion Energy
PRO 1: Science Discovery with ML	PRO 4: Control Augmentation with ML
Hypothesis Generation and	Diagnostics to Data, Dynamic Models for Control,
Experimental Guidance	Fusion Trajectory Design
PRO 2: ML Boosted Diagnostics	PRO 5: Extreme data algorithms
ML Boosted Diagnostics,	Extreme-scale Processing,
Physics Enhanced Data	In-situ Data Analysis
PRO 3: Model Extraction and Reduction	PRO 6: Data-enhanced Prediction
Data-driven Models,	Prediction of Disruption Events and Effects,
Reduction of Complex Code Algorithms	Plasma Phenomena and State Prediction

PRO 7: Fusion Data ML Platform

D. Humphreys et al. "Advancing Fusion With Machine Learning" DOE Workshop (2020)



https://nucleus.iaea.org/sites/ai4atoms/ai4fusion/

Summary and conclusions

- 1. Fusion science and technology advancements accelerated by ML
- 2. ML black boxes can be explained
 - and accuracy does not prevent interpretability!
- 3. Enforce interpretability to reconcile with physics understanding
- 4. Fusion examples already out there employing
 - a. Interpretable algorithms
 - b. Explainable predictions

. . .

- c. Transfer/adaptive learning and statistical optimization
- d. Surrogate modeling for fast reconstructions

Long list of open questions and cross-cutting challenges, but also **opportunities for future research**, **enabling change in the field!**

Reach out if interested in research opportunities at PSFC! <u>crea@psfc.mit.edu</u>





More stuff

Next generation devices will not allow disruption rate > 1% at full performance



Lehnen M. et al 2016 "Plasma disruption management in ITER", 2016 IAEA Fusion Energy Conf. EX/P6-39 Reproduced at E. Strait et al Nucl. Fusion (2019) 112012



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A simple, interpretable, and accurate model *should* exist, maybe (computationally) hard to develop

Supervised and interpretable ML classification workflow:



Examples of explainable models interpretable by design



Physics-informed machine learning seamlessly integrates data and governing physical laws

- NN and AutoDiff allow to design models with partially missing physics (or data!)
 - No need of domain adaptation or transfer learning.
 - Strong generalization, by enforcing/embedding physics constraints.
 - Can tackle high-dimensional problems.
 - Can address uncertainty due to physics, data, and learning models.



Physics Informed Neural Networks (PINNs) preserve interpretability through physics constraints

• PINN learns partial differential equations (PDEs) given initial and boundary conditions (I&BC): heat equation example.



- PINN training minimizes the PDEs residuals + I&BC, through combined loss function and automatic differentiation.
- No need of labeled data, only generative constraints!

Adapted from: C. Rudin et al., 2022 Stat. Surv. 16 1–85 G.E. Karniadakis et al., 2021 Nat Rev Phys 3, 422–440

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PINN solves heat equation and computes heat flux on the top surface of W7-X divertor tiles



PINNs can accurately learn turbulent field dynamics consistent with theory, and from partial observations



A. Mathews, et al, Phys. Rev. E 104, 025205 (2021)

PINN reconstructions

60 Explainability vs interpretability

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Physics-informed machine learning: current limitations

- Multiscale and multiphysics problems require further developments.
 - High-frequency functions difficult to learn \rightarrow F-principle or spectral bias.
- PI ML involves highly non-convex optimization problems for complex loss functions.
 - Need more robust algorithms and computational frameworks.
 - Meta-learning techniques to automate the design of best architectures?
- Missing benchmarks on openly available datasets from physics, chemistry, ...
- More research needed on the theoretical foundations of NN.

G.E. Karniadakis et al., 2021 Nat Rev Phys 3, 422–440 and references therein

Domain adaptation and transfer learning: ML mapping from inputs to outputs, or learning to perform a task

Simplified supervised ML classification workflow:

Adapted from A. Pau et al, Nuclear Fusion, 59(10):106017, 2019



• Mapping from inputs to outputs through ML systems means to learn to perform a task.

Learning a task heavily depends on dataset composition

- What if the collected data is **not an accurate reflection of the population**? Too limited, not accurately labeled, ...
 - Learning a general data representation by finding common embeddings of source/target data!



Domain adaptation and transfer learning designed to overcome biased dataset and/or generalize knowledge across different tasks.

Data Augmentation: brief background



Ideal Conditions



More (non-disruptive) examples:

Temporal Convolutional Neural Network predicts confinement probability 1ms in the future



Neural networks accelerate equilibria reconstructions and profile evolution for shot planning and real-time control



Gaussian Processes (GP) enable nonlinear simulations for performance prediction and gyrokinetic validation

- Few (10-20) simulations required to reach convergence, thanks to Bayesian Optimization (BO) workflow + GP surrogate modeling.
- Enabling profile predictions of unprecedented accuracy for:
 - Prediction of burning plasma performance (e.g. SPARC)
 - ✓ Validation of gyrokinetic codes (e.g. DIII-D)



Solution

P. Rodriguez-Fernandez et al, Nucl. Fusion 62 (2022) 076036

Open question: detangle local minima from unique physical solutions



Raw ECE time series input data to Reservoir Computing Network to compute Alfvén Eigenmode score



Jalalvand et al 2022 Nucl. Fusion 62 026007







True Positive Rate: **%91** False Positive Rate: **%7**

> caution: how sensor failures affect ML workflow accuracy

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Decision paths in RF trees provide local measures of explainability through information gain and loss



Source domain (simulations) allows to learn how to reconstruct target data (experiments)



Fusion

- Large datasets built through inexpensive but possibly inaccurate simulations.
- Networks (autoencoders) trained to learn mapping between sim-to-sim inputs to outputs.
- Mapping then transferred to new task → learning corrective transformation mapping sim-to-exp → transfer learning!

Adapted from Humbird et al., PoP 28, 042709 2021

Transfer learning

Improving instability avoidance with data-driven analysis of the "density limit"

- Density limit critical for ITER, but standard "Greenwald Limit" not sufficiently reliable
- Our study identified novel equation

$$\frac{n_{\rm edge}}{T_{\rm edge}^{0.79}} = 3 \cdot 10^{-3}$$

outperforms Greenwald, other benchmarks, in predicting density limit at DIII-D

• Expanding to multi-machine database





Andrew Maris, maris@mit.edu
Disruptions modeled as Poisson processes with characteristic time 1/disruptivity (1/s):

 $P(k \text{ disruptions in } \Delta t|d) = \frac{(d\Delta t)^k e^{-d\Delta t}}{k!}$

 $P_D(\Delta t|d) = 1 - e^{-d\Delta t}$

probability of disruption in the next Δt (s)

P. Kaloyannis (EPFL), C. Rea, 2023 Master's thesis



