Digital Twins and Surrogate Models for Efficient Interplay Between Fusion Experiment and Simulation

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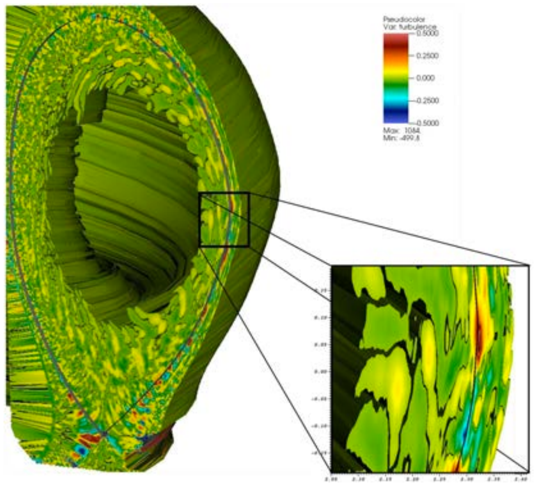
**Oak Ridge National Laboratory*

Introduction

- A brief introduction to magnetic fusion science, which is in need of digital twins and surrogate models
- Fusion workflows: present and future
- Role of digital twins and surrogate models
- Example surrogate twins and surrogate models
- Summary



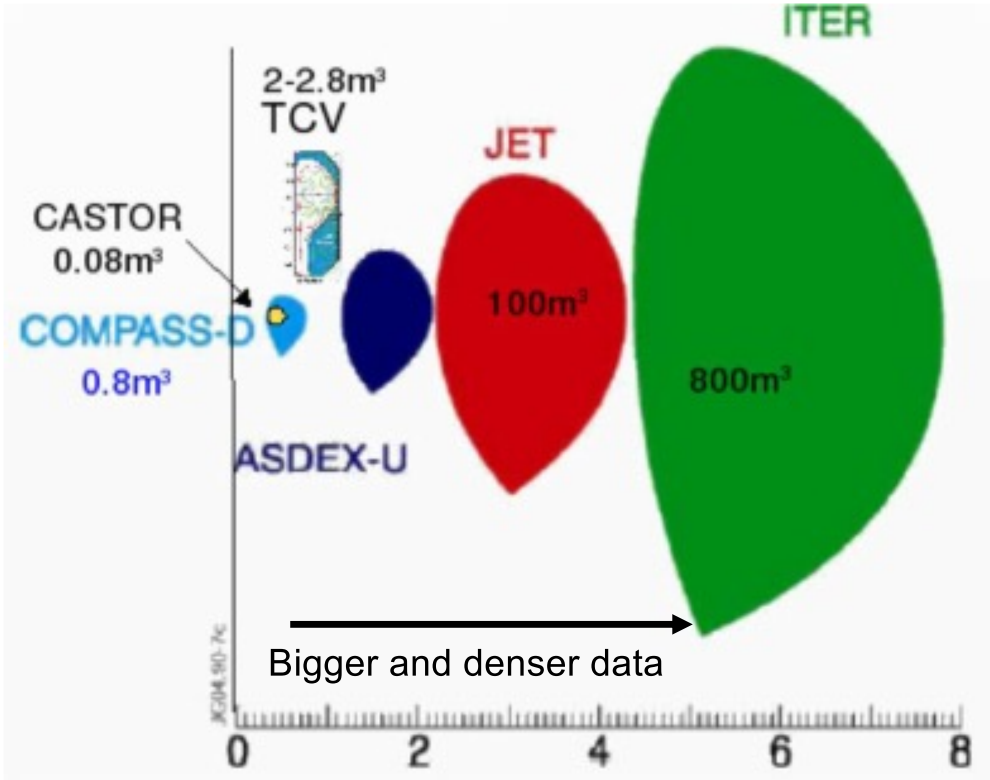
My personal definition of DT/SM used in this talk

- Digital Twin (DT): Physics based model; good in the parameter-space represented by physics equations
- Surrogate Model (SM): Data based model; good in the parameter-space represented by data, but not covering the space represented by equations
- DT and SM need to be fast enough for the time-scale they are aiming at.

Magnetic Fusion Science

- Enable fusion reactor operation using magnetically confined plasma
  - Little environmental and safety issues compared to nuclear reactors
  - Carbon-neutral fuel: nearly inexhaustible deuterium, distilled from water
- Long enough confinement of D-T plasma at ~15keV is key
  - Confidence from existing experiments led to construction of ITER with 10 times return energy on investment energy
  - Higher-fidelity **simulation** is needed to reduce uncertainty, accelerate progress, and lower cost
  - Scientific difficulty: nonlinear, nonlocal, multiscale self-organization of multi-physics

→ Big and dense data from simulation and experiment that interact in multiscale

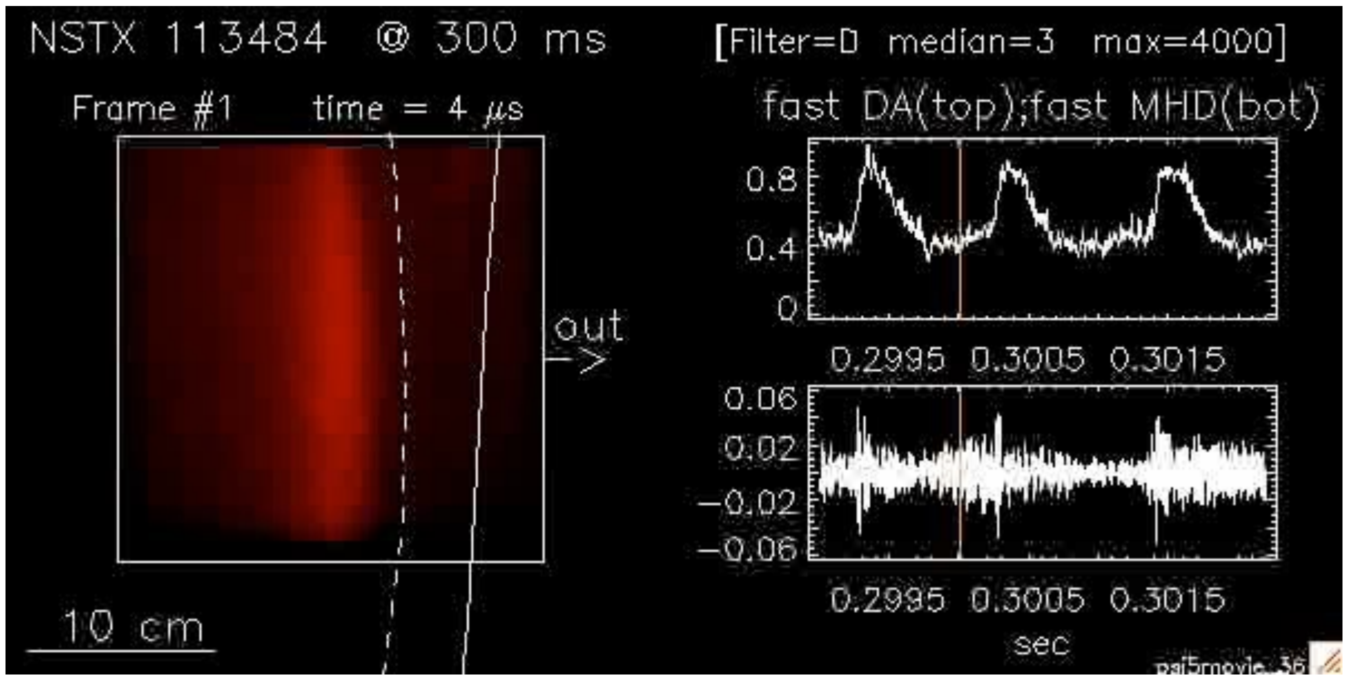


Tokamaks are getting bigger and the diagnostics is getting denser, so are the data.

Catastrophic instabilities (~ms)

- Fusion reactors need to control/mitigate two catastrophic global instabilities that can cause structural or material damage
  - Eedge localized modes (ELMs) and
  - disruptions

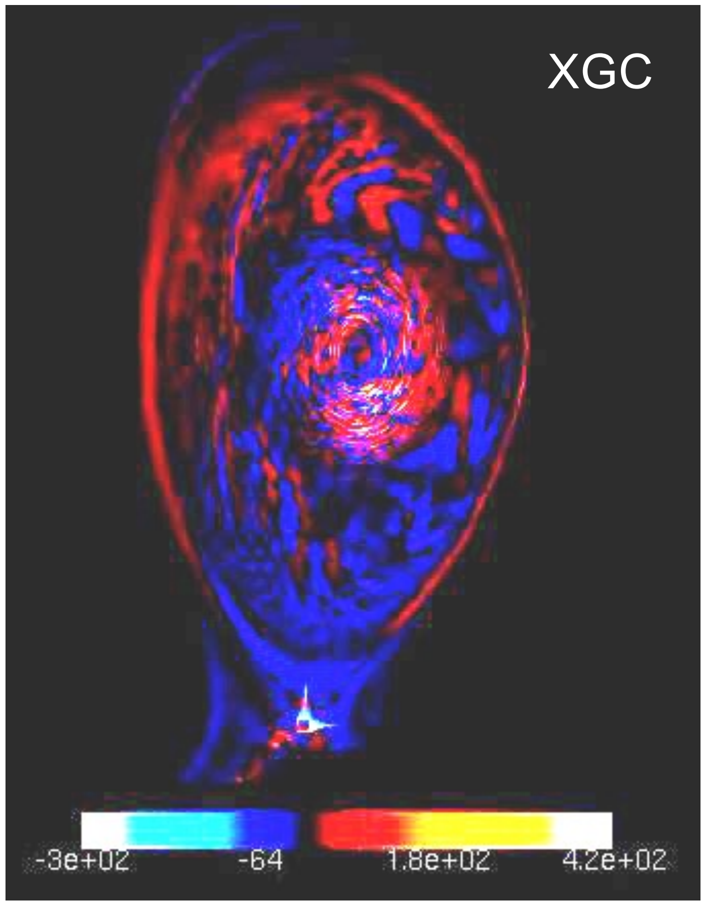
Edge Localized Mode (**ELM**) crash in NSTX-U tokamak



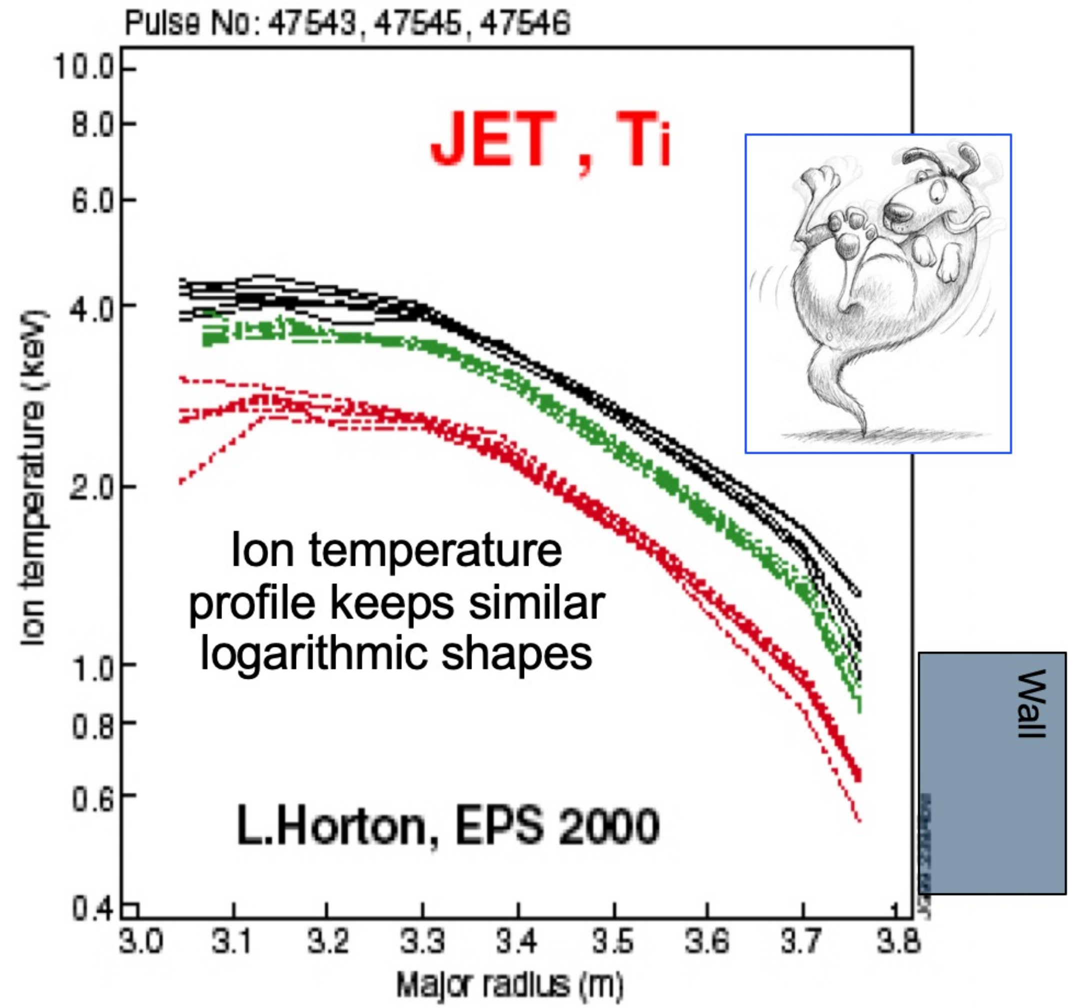
A plasma **disruption** event in C-Mod tokamak

Transport timescale physics (~ms - s)

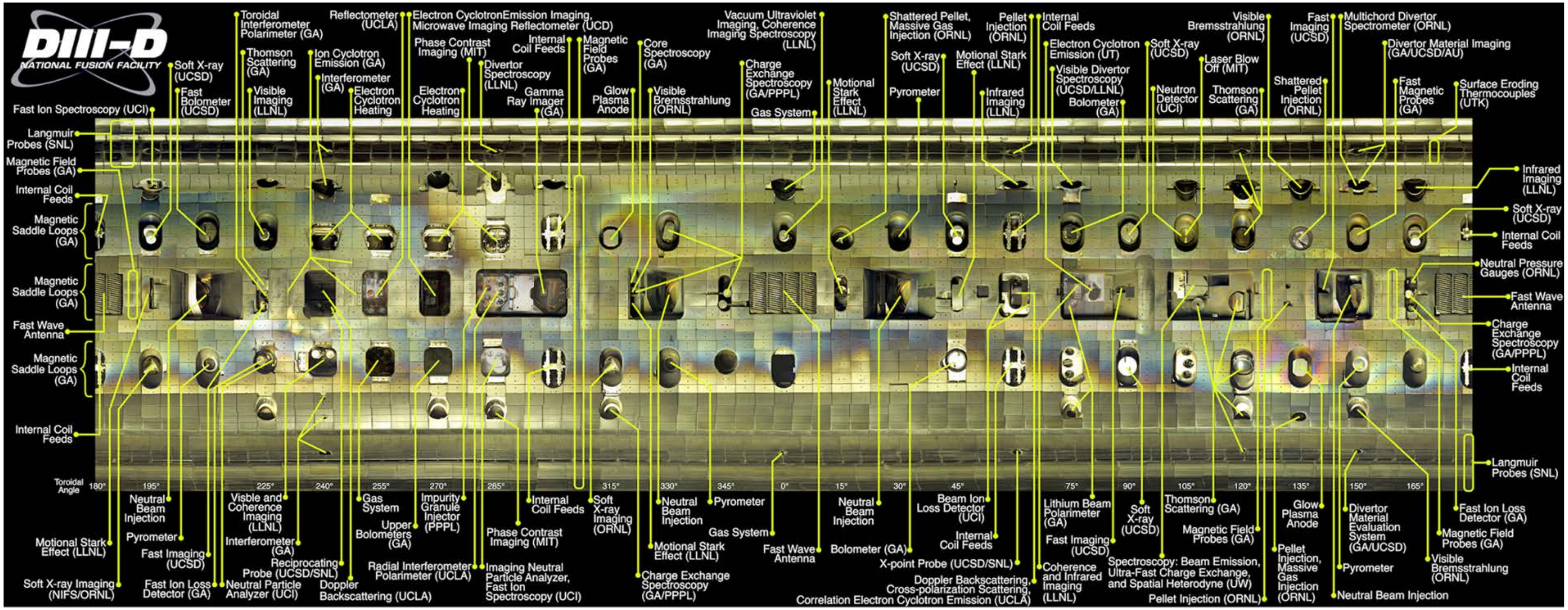
Turbulence and particle orbit dynamics determines the confinement and is nonlocal & multiscale.



The tail wags the dog.



Hundreds of diagnostics with thousands of sensors are utilized on tokamaks to study multiscale Multiphysics plasma behavior



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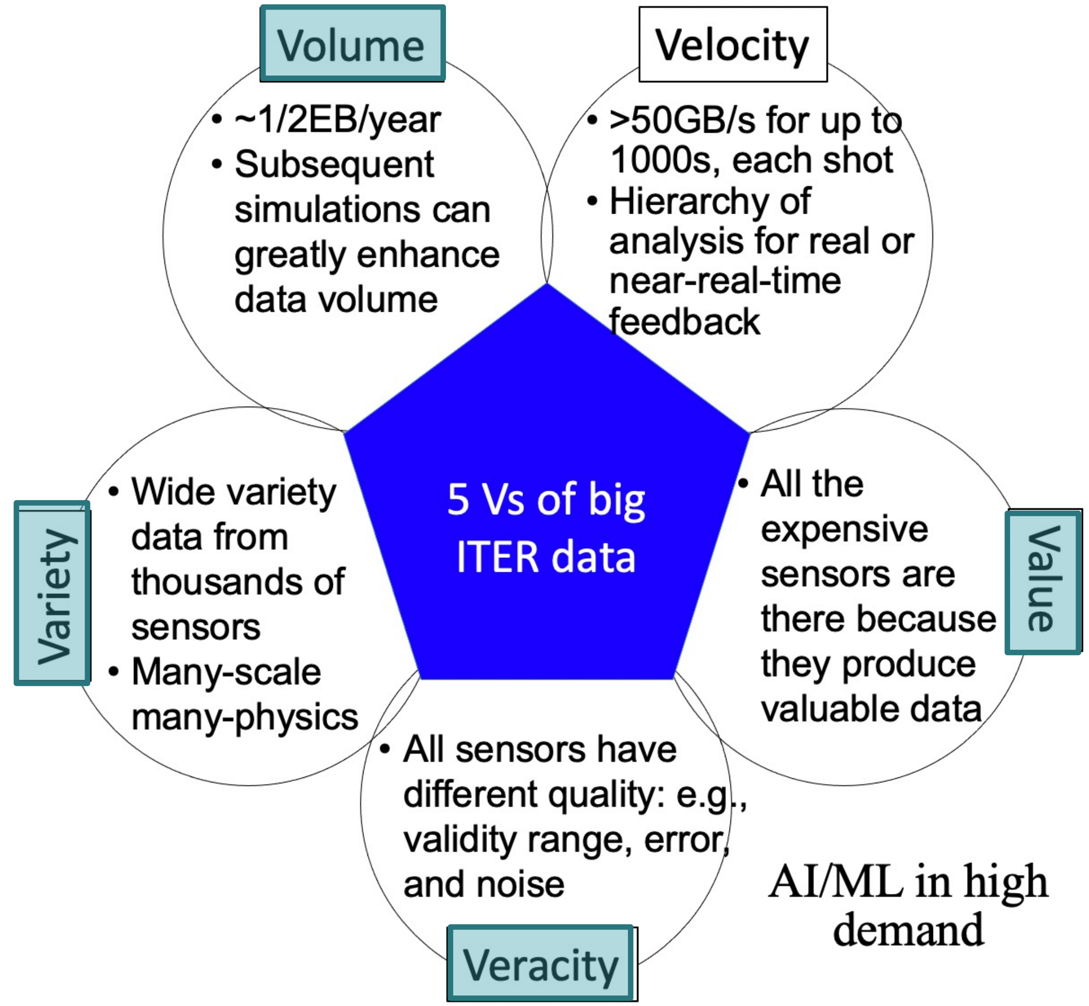
Data challenge in Fusion Science

It is all about big 5Vs.

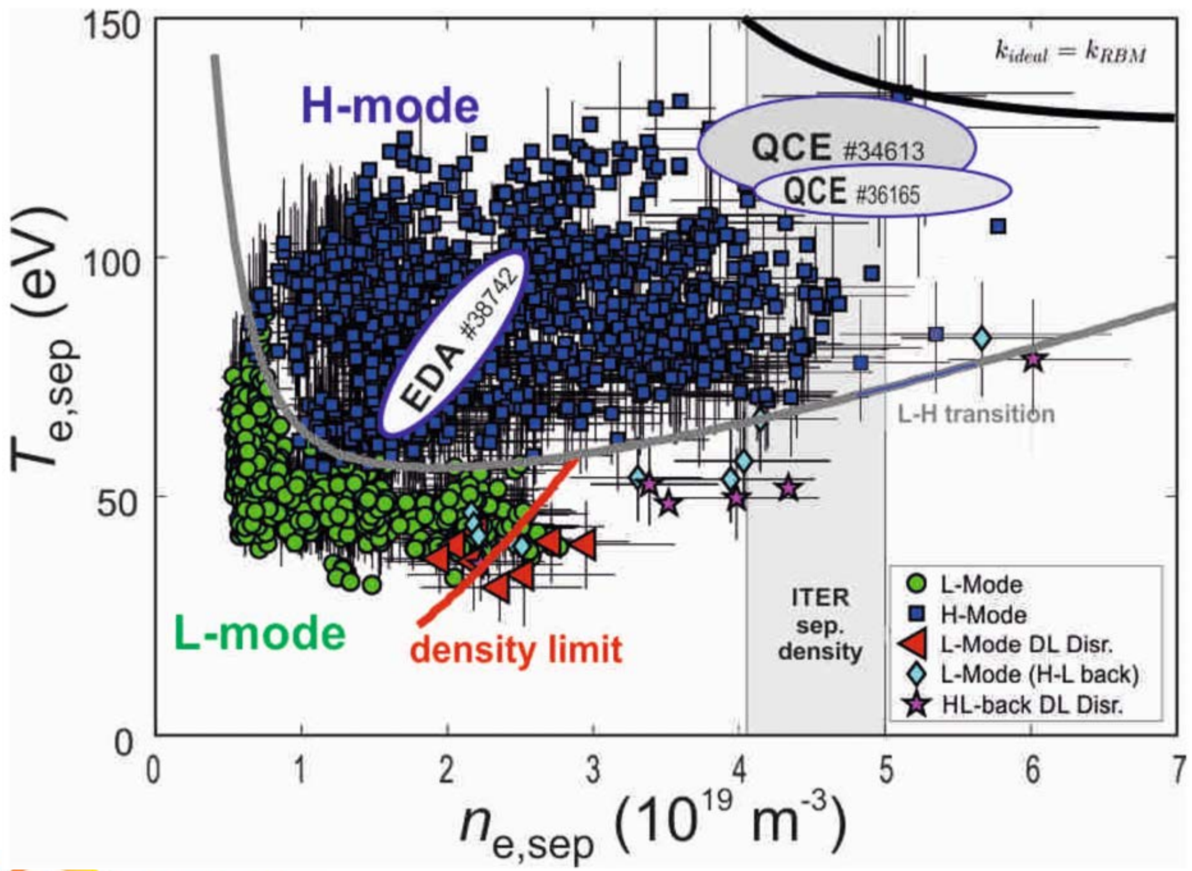
- **ITER is under construction**, we need to get ready
  - Data is dense with a serious accumulation speed. **Smart in-line reduction/analysis is needed,** meeting different requirements
- Design of next fusion reactor is starting now: relies on Digital Twins & Surrogate models built from predictive simulations
- **Exascale computers** will play important role, but
  - Simulation data will be **~Exa-Bytes per day**
  - Simulation steering needed, not to waste expensive computing resources
  - Various synthetic diagnostics data from simulation and thousands of sensors from experiment need to get married with **dynamic multiscale interaction** in mind for proper digital twins & surrogate models.



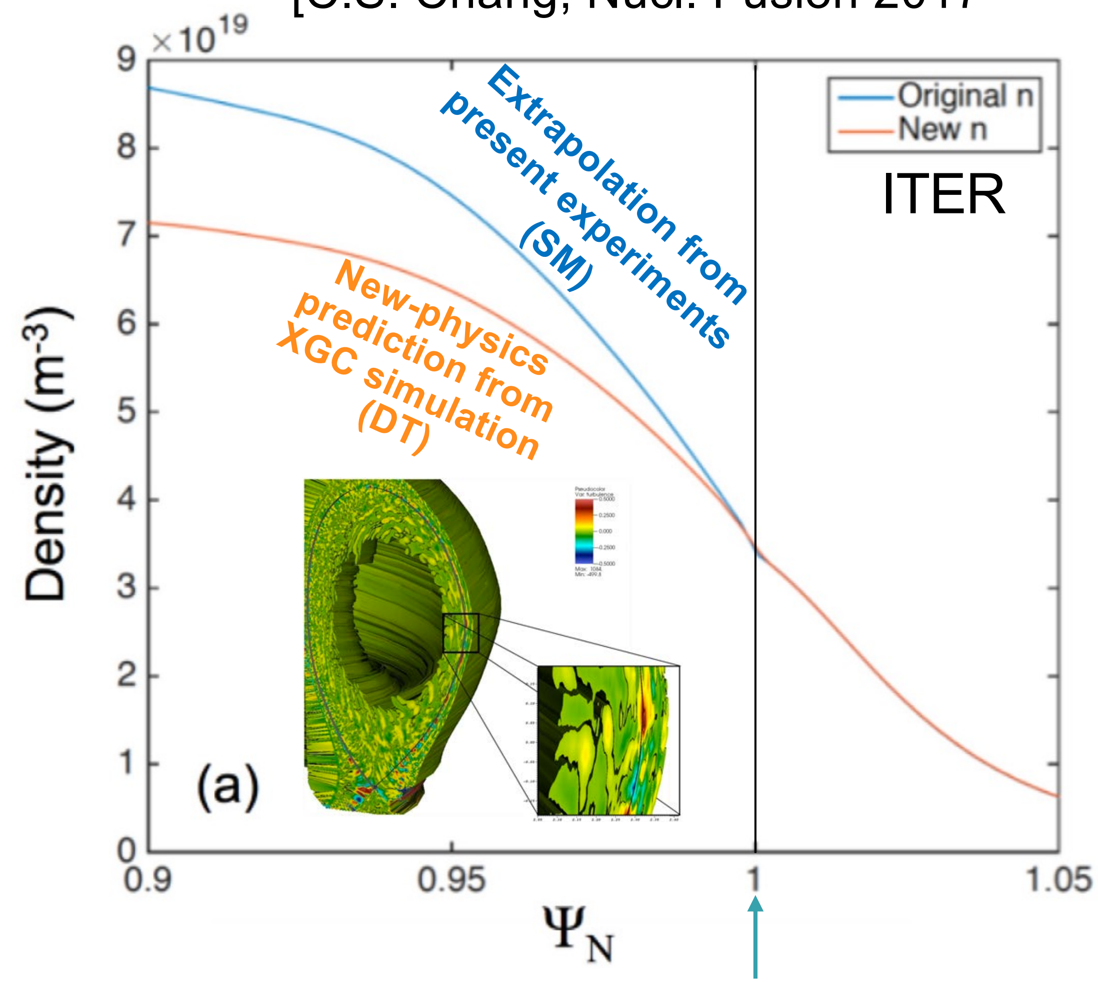
Dense fusion data can quickly accumulate to an uncontrollable level.

Most of the physics is determined by the edge plama parameters, giving hope to simplified Digital Twin and Surrogate Model construction/application since the number of knobs could be small.

Separatrix plasma determins operational boundaries
[U. Stroth, IAEA-FEC2020]

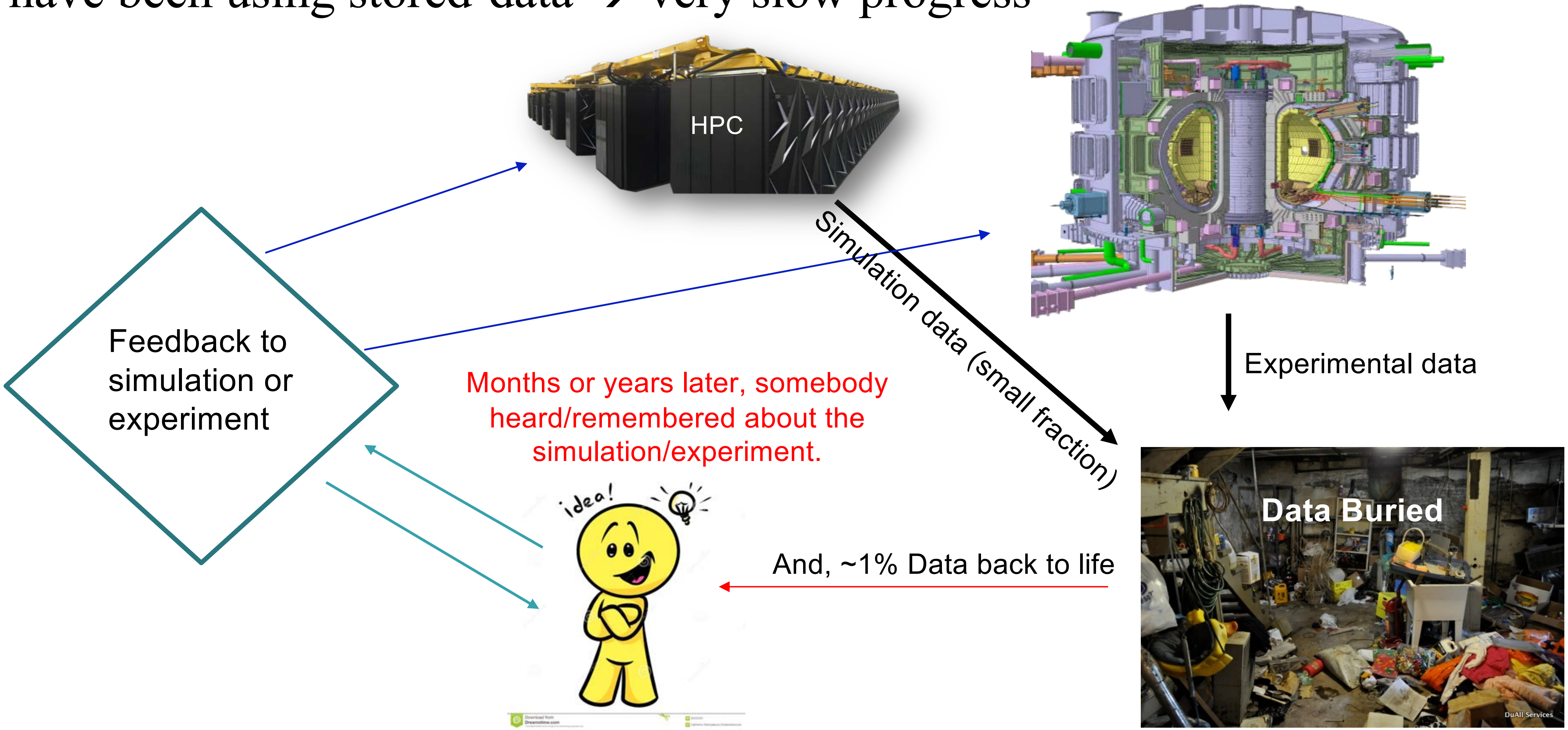


[C.S. Chang, Nucl. Fusion 2017



What is the present science-workflow?

We have been using stored-data → very slow progress



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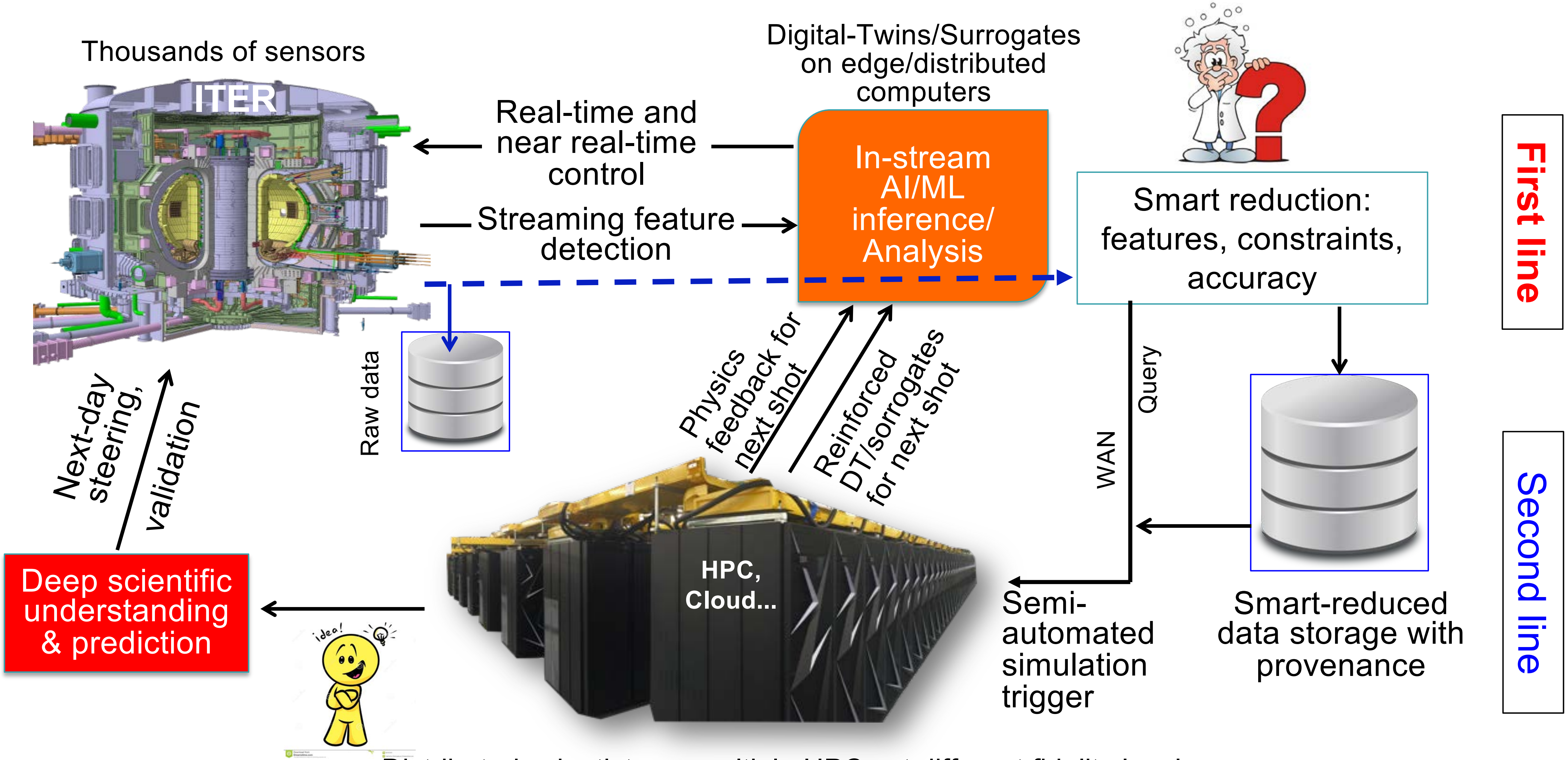
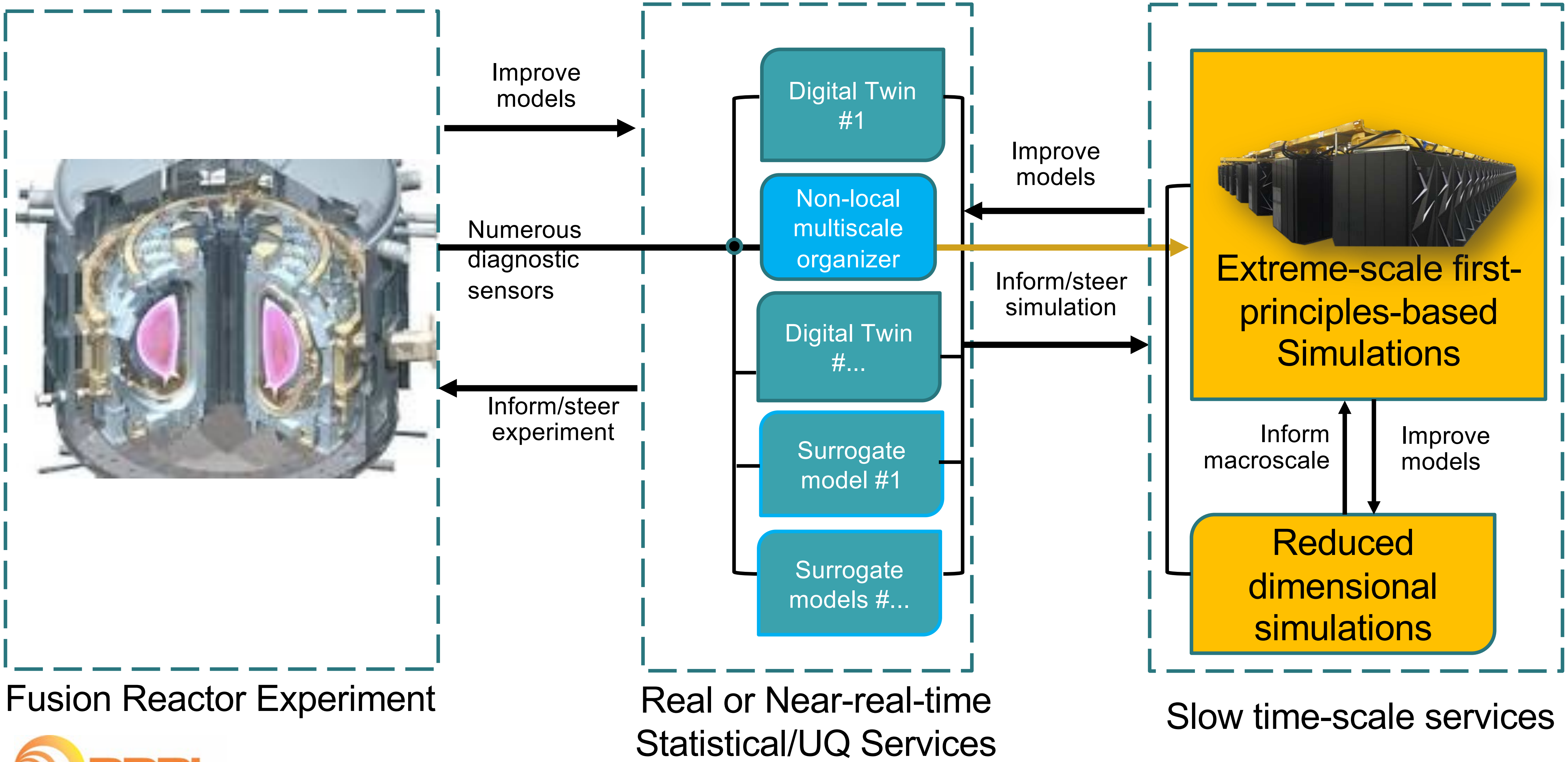
Future workflows for accelerated science: automated or semi-automated

(timescale from months/years to real-time/days)



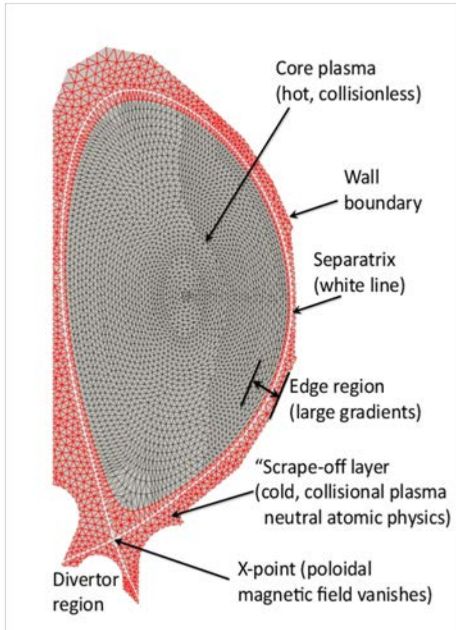
Distributed scientists on multiple HPCs at different fidelity level.
Real time simulation steering.

Digital-Twin/Sorrogate Services in our vision

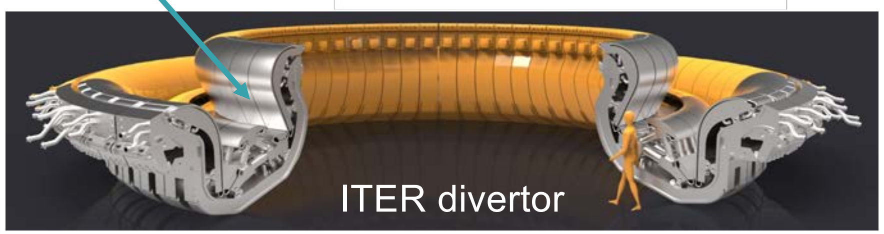


Examples of Digital Twin and Surrogate Model Construction

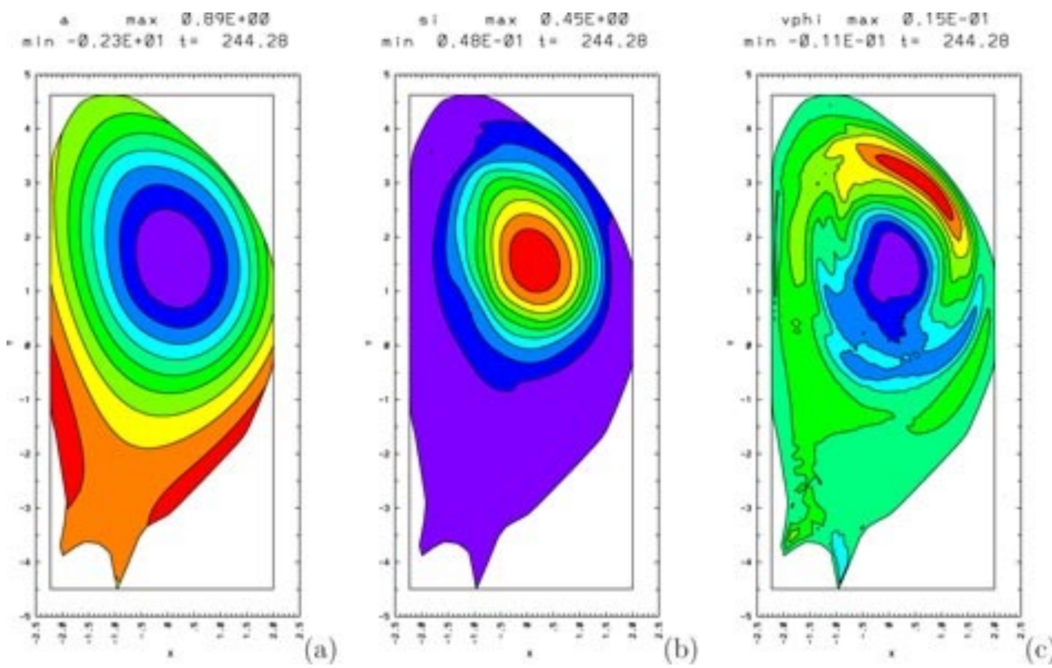
- **Digital Twin example**: power density from heat-exahust on divertor plates
  - The heat-load power density should not exceed material tolerance limit.
- **Surrogate Model example**: Prediction for major disruption
  - A mitigation actuator must be triggered before the reactor wall/structure are damaged.



Tungsten plates



A major disruption instability quickly dumps the entire plasma energy/current to wall/structure.



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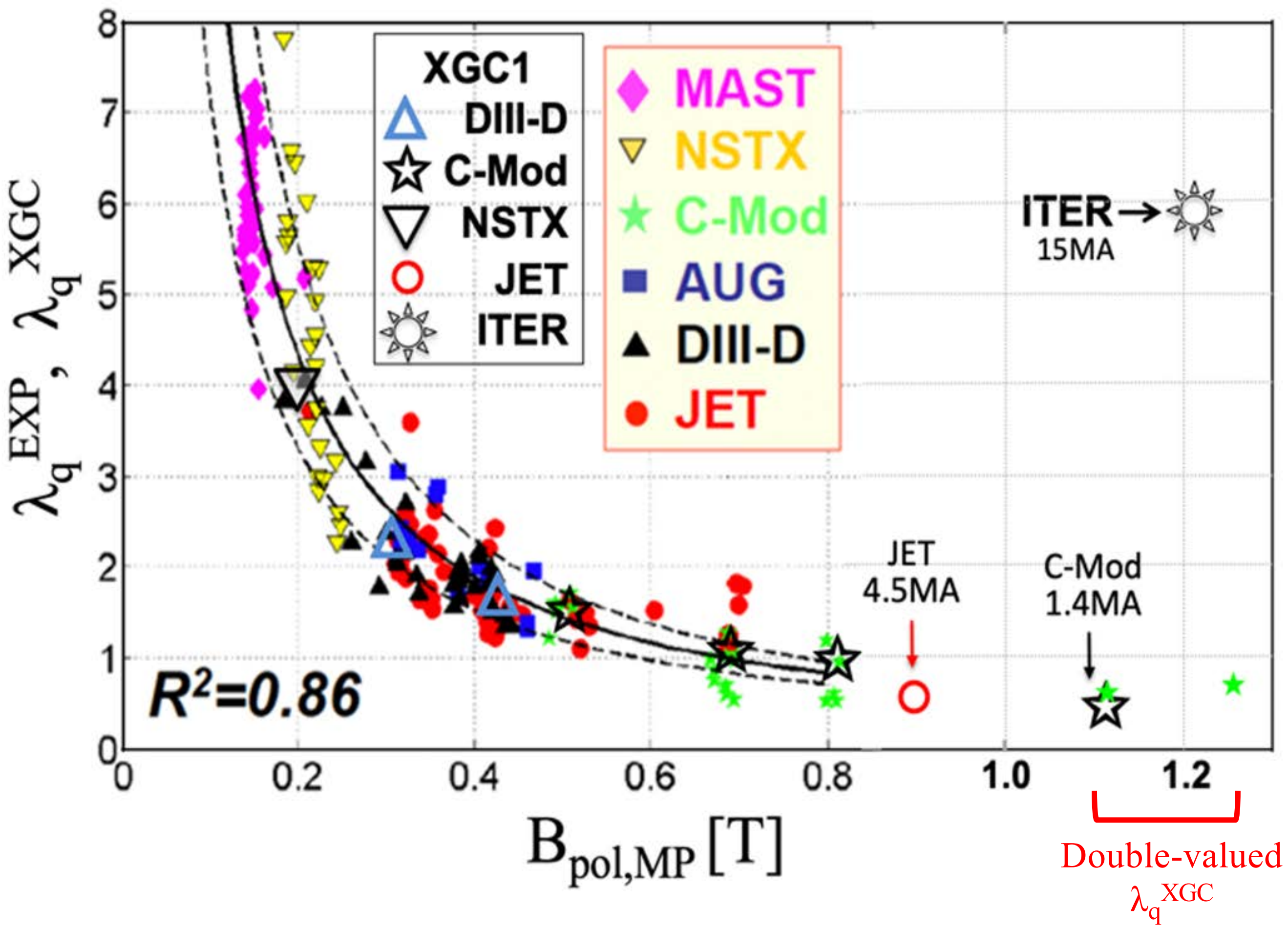
XGC that predicted λ_q^{XGC} values in agreement with experimental $\lambda_q^{Eich(14)}$ in all three US tokamaks and JET predicted $\lambda_q^{XGC} >> \lambda_q^{Eich(14)}$ in the full-current ITER plasma



Solid line: Experimental $\lambda_q^{Eich(14)}$
Dashed line: Eich(14)'s regression error

Experimental data is for interpolation → A non-physics based extrapolation could be dangerous.

- λ_q solution from XGC is double-valued around 1.2MA
- Hidden parameter that was not included in Eich's regression?
  - The important kinetic parameter ρ_i/a is missing in Eich's parameter set.
- How can we verify if ρ_i/a can resolve the double valuedness?

  → A new simulation-anchored regression study or "Simulation-Anchored ML"

Figure from C.S. Chang et al., Phys. Plasmas 28, 022501 (2021) https://doi.org/10.1063/5.0027637]

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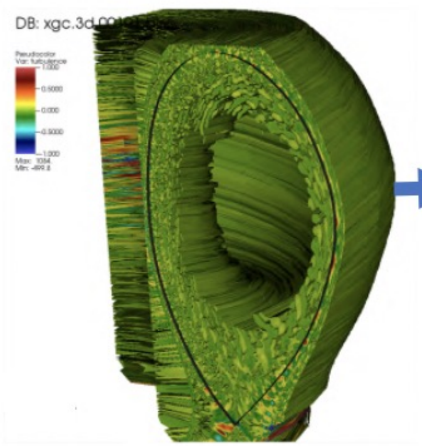
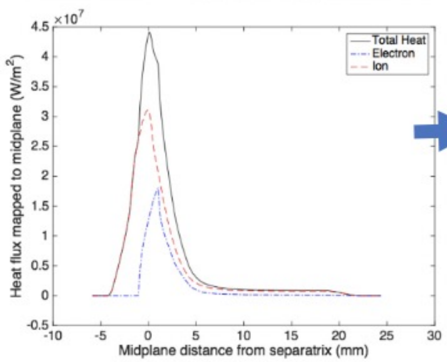
We utilized the supervised AI/ML program Eureqa#

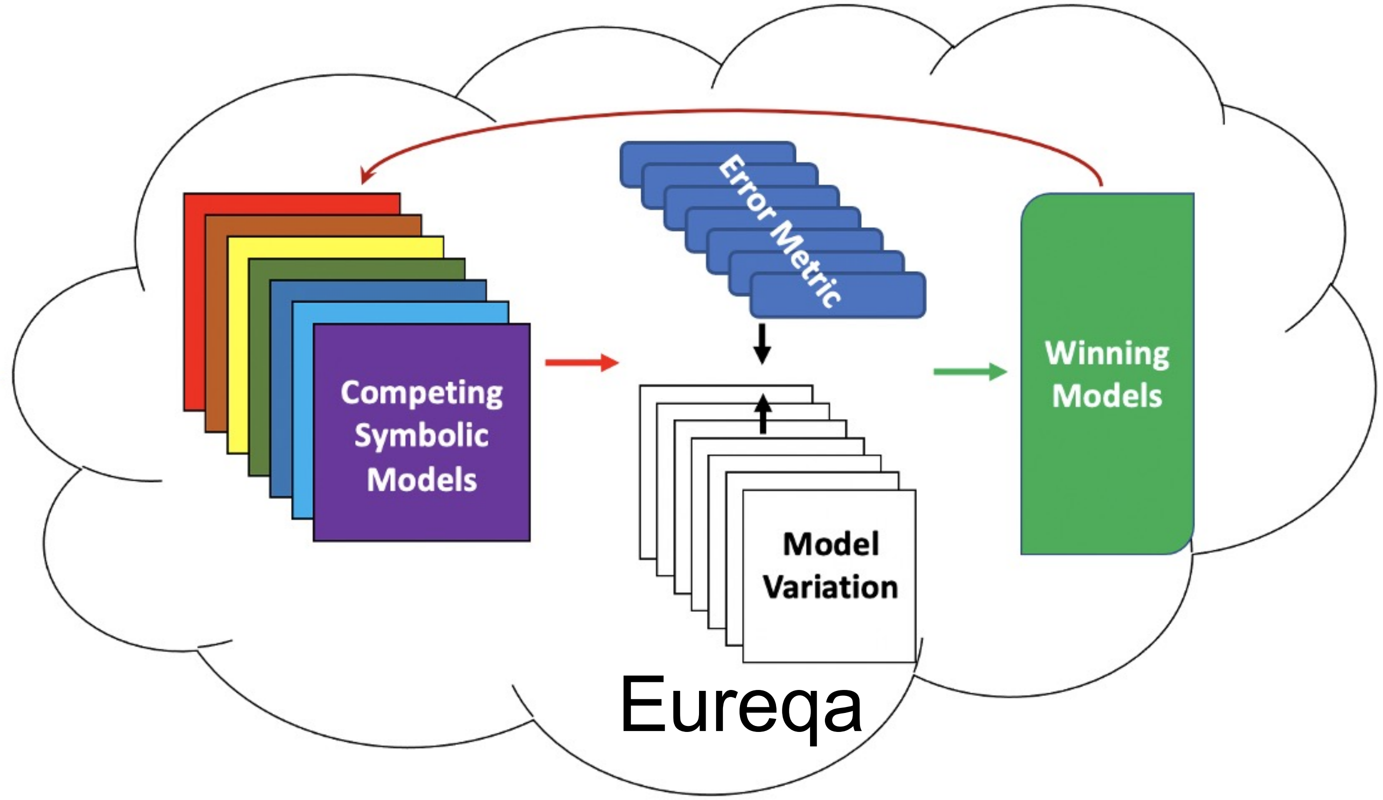
Physics informed Supervised learning





- Labeled data
- Mathematical Building blocks
  - +, -, x, /, 10^{x+y}, x^k, y^k, x^y, …
  - $f(B_{pol,MP}, a/\rho_{i,pol})$, $f(B_{pol,MP}, a/\rho_{i,pol}, B_{pol,MP}\, a/\rho_{i,pol})$, $f(B_{pol,MP}\, a/\rho_{i,pol})$

Inputs for supervised learning

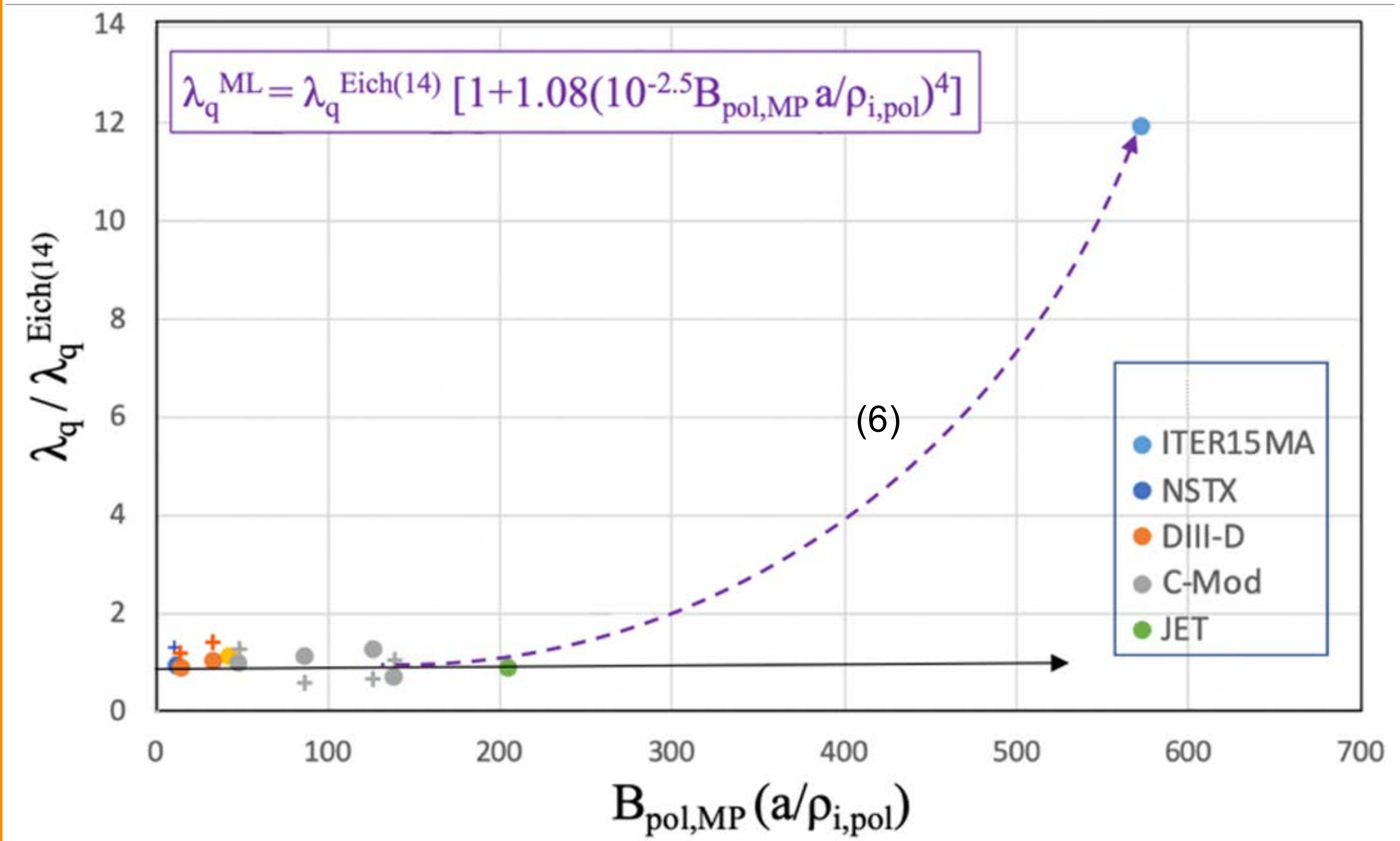


Evolutionary Model search

$$\lambda_q^{ML} = 0.63 B_{pol,MP}^{-1.19} [1.0 + 1.961\times10^{-16} (a/\rho_{i,pol})^6]$$

#An AI-powered modeling engine by Nutonian (https://www.nutonian.com/products/eureqa/); now acquired by DataRobot

The AI program Eureqa suggested several simple formulas



Here, $\rho_{i,pol}$ represents ion temperature on **separatrix**.

λ_q^{ML}=0.63$B_{pol,MP}^{-1.19}$ [1.0 + 1.08x10^{-10} ($B_{pol,MP}$ a/$\rho_{i,pol}$)^4] with RMS error=18.7% (6)

=0.63$B_{pol,MP}^{-1.19}$ [1.0 + 1.961x10^{-16} (a/$\rho_{i,pol}$)^6], RMSE=17.9% (7)

=0.63$B_{pol,MP}^{-1.19}$ [1.0 + 1.68x10^{-18} $B_{pol,MP}$ (a/$\rho_{i,pol}$)^7], RMSE=17.0% (8)

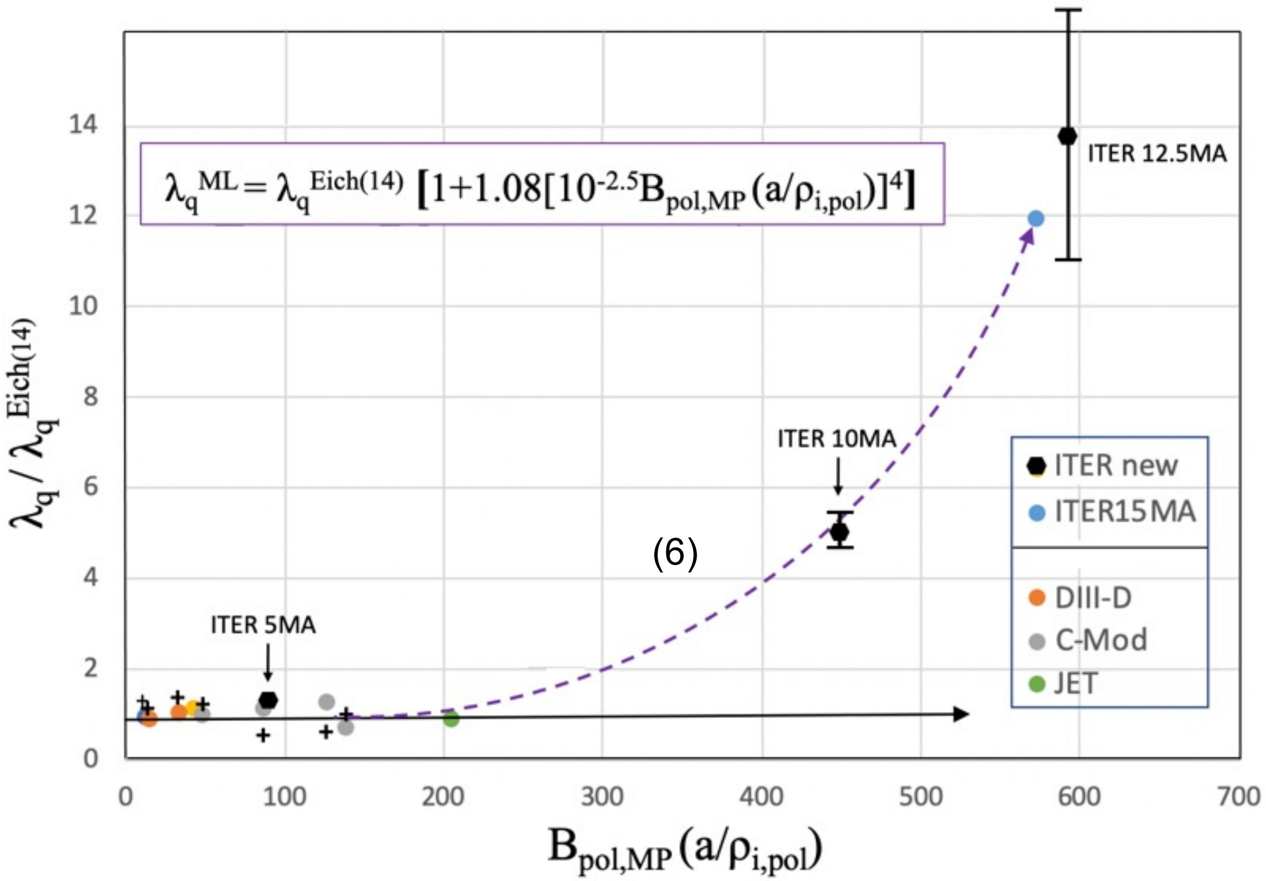
=0.63$B_{pol,MP}^{-1.19}$ [1.0 + 1.91x10^{-13} ($B_{pol,MP}$ a/$\rho_{i,pol}$)^5], RMSE=17.0% (9)

=0.63$B_{pol,MP}^{-1.19}$ [1.0 + 3.46x10^{-4}[4.04x10^{-5} $B_{pol,MP}$ (a/$\rho_{i,pol}$)^3]$^{B_{pol,MP}}$, RMSE=16.1%. (10)

Which one should be taken?

The simplest one works the best (see next page).

We have tested the formulas with three more ITER simulations. The simplest formula works the best when compared to XGC result.



Formula No.	λ_q^{ML} from various formulas	Ratio to λ_q^{XGC}=2.65mm
Eq. (6)	2.77 mm	1.05
Eq. (7)	0.86 mm	0.32
Eq. (8)	1.79 mm	0.68
Eq. (9)	2.30 mm	0.87
Eq. (10)	2.24 mm	0.84

- What could be the new physics?
- Is a/ρ_i really different between ITER and the present-day tokamaks and the ExB shearing rate really dependent on a/ρ_i?

- At $\lambda_q \sim 12\lambda_q^{Eich(14)}$, ITER operations can be much easier, possibly leading to faster scientific progress.
- This simple formula can be tested on ITER and, if **validated**, can be used for reactor design.
- Can it be validated on today's tokamaks and utilized for ITER's operation scenario development with higher confidence?

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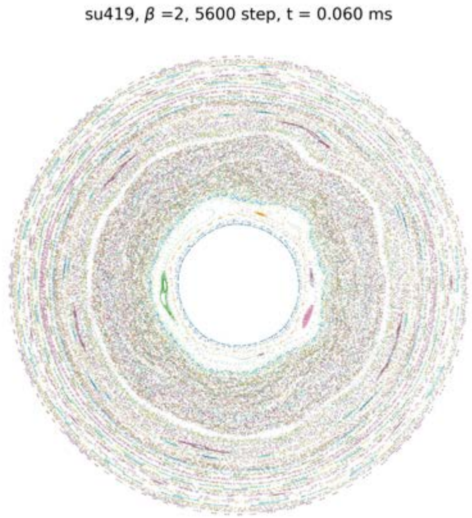
Example: Surrogate Model Construction for Disruption Prediction using Deep Convolutional Neural Networks

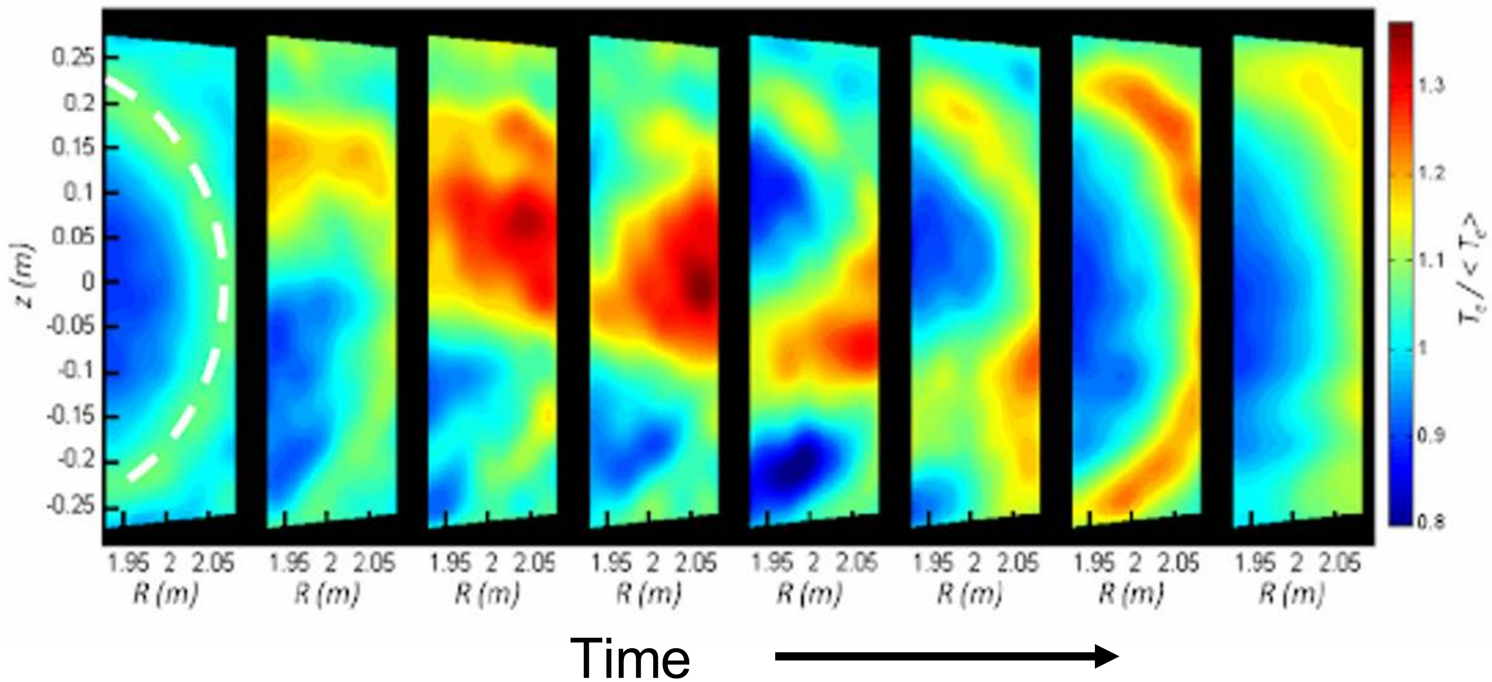
- The goal is to utilize higher dimensional and muitiscale multiphysics data to raise the reliability
  0D → 1D → 2D (present) → 3D and edge plasma data (future)

Growth of magnetic islands could be related to disruption trigger.

[3D XGC simulation, S. Ku et al.]



2D Electron Cyclotron Emmision Imaging (ECEI) data from DIII-D



[B. Tobias et al., RSI (2010)]

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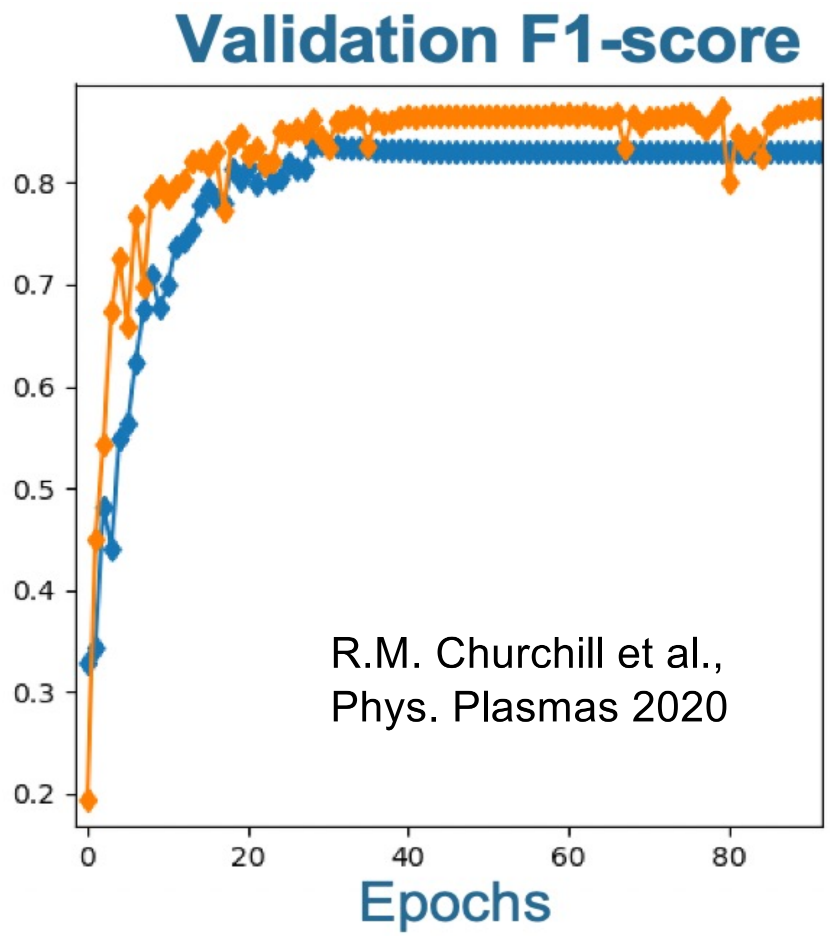
86% reliability can be obtained from this 2D CNN surrogate-model



- Mimimum wanring time for ITER is ~30ms
- Future work to raise the F1-score
  - Incorporate other relevant diagnostics data (e.g., edge data)
  - Utilize physics understanding and information from first-principles-based simulations → digital twin

Summary

- Magnetic fusion physics is too complex (nonlocal, nonlinear, multiscale, multiphysics in complicated and inhomogeneous geometry) to be understood/predicted without running first-princeples-based simulations on HPC computers
- Extreme-scale computing cannot be utilized for real-time or near-real-time progress
- Human-in-the-loop has been making the experiment-HPC interaction to be months or years
  - Requires automated or semi-automated workflows with fast ditigal twins (DTs) and/or surrogate models (SMs) on edge computers
  - Fortunately, there are only handful of knobs that govern the time-asymptotic solution
- The magnetic fusion community is working towards DTs and SMs for
  - Prediction of catastrophic instability events (disruption and edge localized modes)
  - Divertor wall-load of exhaust heat
  - Plasma transport and profile evolution, and others
  - Redeced model whole device/physics frameworks exist, but not yet fast enough to be called DT/SM.
- A strong collaboration with AI/ML and Data Management communities are being pursued.
  - Data reduction, feature detection, physics conservation, service framework, …

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