Integrated multi-physics modelling for tokamak plasma science

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- Brief domain introduction to tokamaks
- Challenges in integrated tokamak plasma simulation
- Case studies: JET tokamak W-impurity predictions
  Neural network surrogate models for plasma turbulence

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Short Bio

- Since 2016, heads DIFFER group "Integrated Modelling and Transport".

  Part-time Associate Professor Eindhoven University of Technology

- PhD Eindhoven University of Technology 2012

  Postdoc CEA/IRFM 2013-2016

- Selected research themes:
  - Integrated tokamak modelling – mostly within EUROfusion consortium
  - Tokamak turbulent transport; co-developer QuaLiKiz code (www.qualikiz.com)
  - Surrogate modelling with neural networks for simulation acceleration


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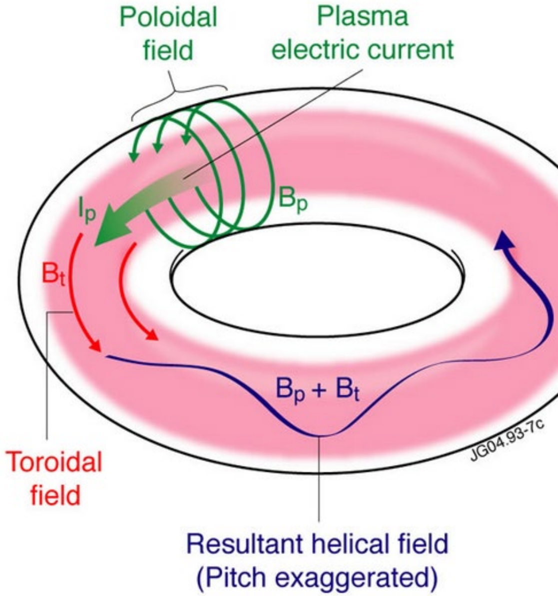
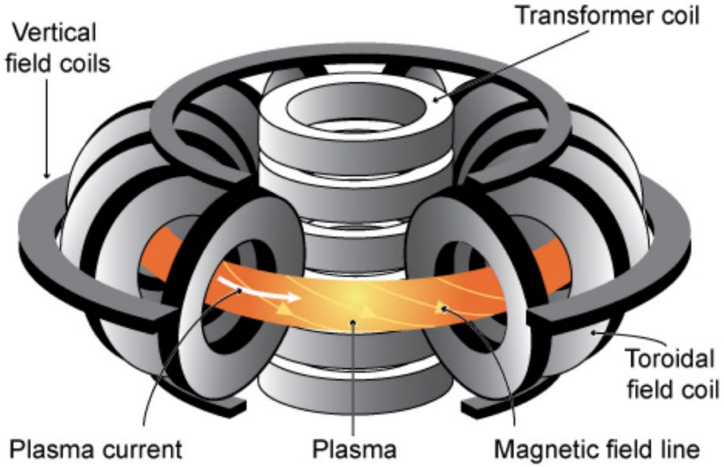
The "tokamak" is the leading design for achieving controlled fusion energy reactors

Plasma configuration



Magnetic coil configuration



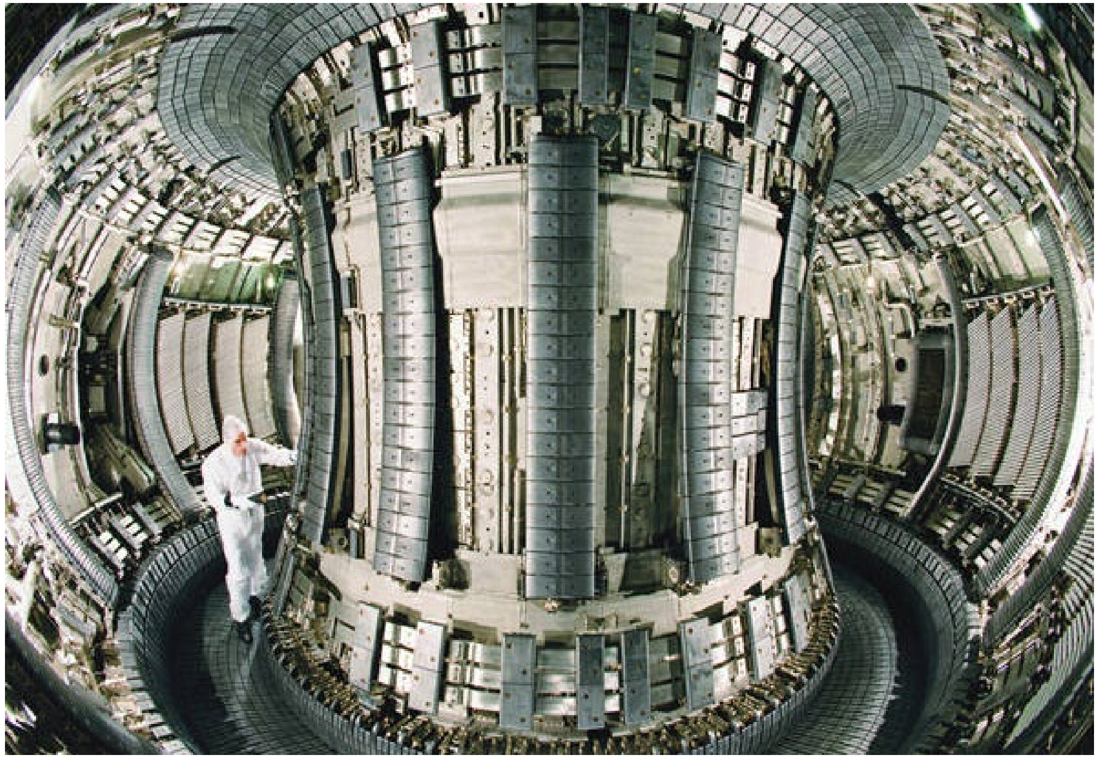
- Helical magnetic field needed to achieve confinement
- Toroidal axisymmetry → unperturbed particle trajectories confined.

  Energy losses due to perturbations from instabilities and turbulence!
- Typical parameters: R = 2 m, B = 5 T, T = 20 keV ($\sim 10^8 K$), n = 10^{20} m^{-3}
- Plasma heated to fusion conditions by radiofrequency waves and accelerated beams

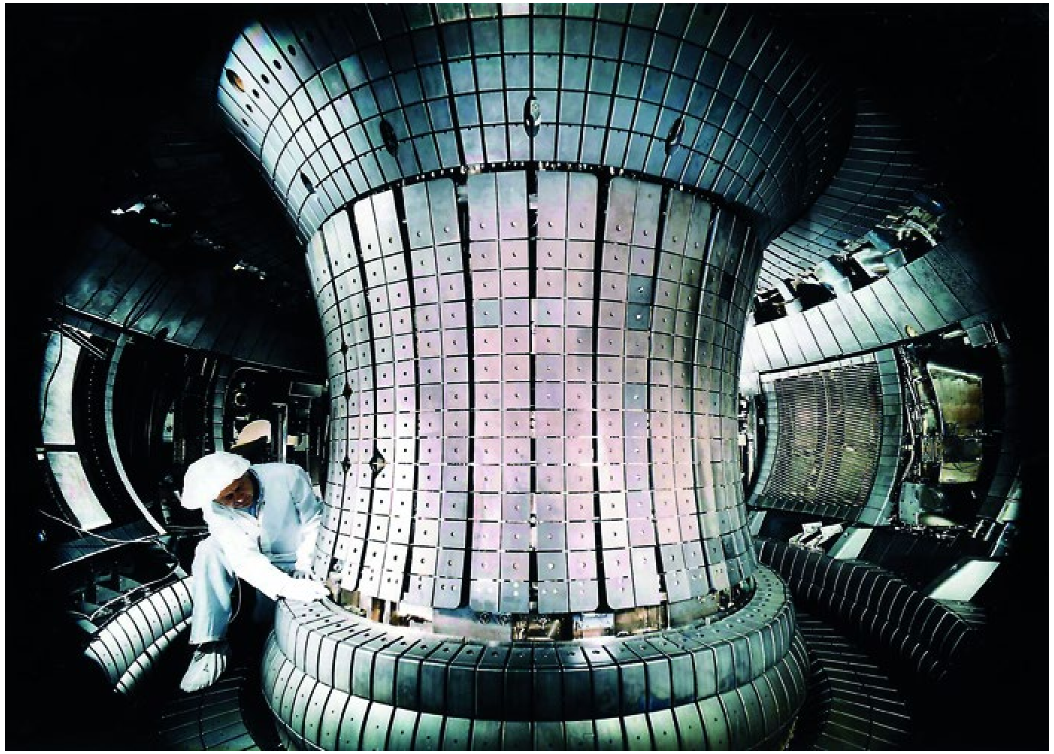
Impression of present-day tokamak experiments

Originated in USSR in 1960s.
Multiple experiments worldwide: illustration of largest EU devices

Joint European Torus (JET), Culham, UK



ASDEX-Upgrade
Max Planck Institute for Plasma Physics, Germany



Next generation of experiments to achieve net fusion gain for first time

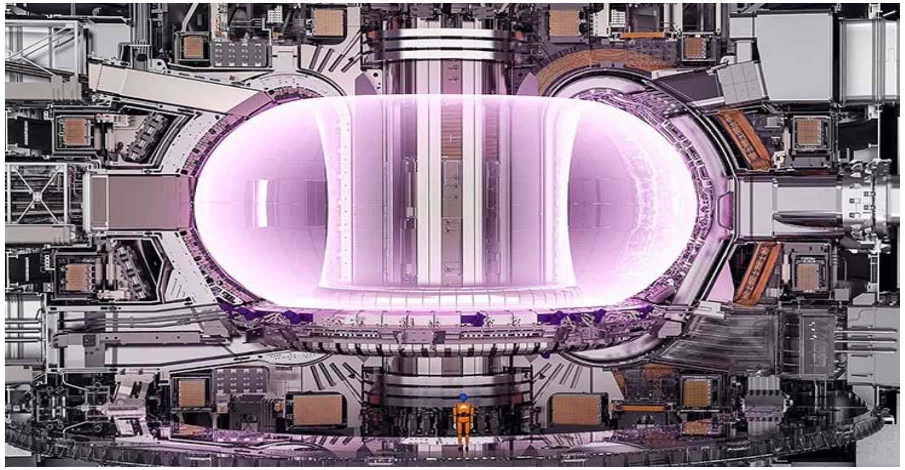
ITER construction in Cadarache, France

Credit © ITER Organization, http://www.iter.org

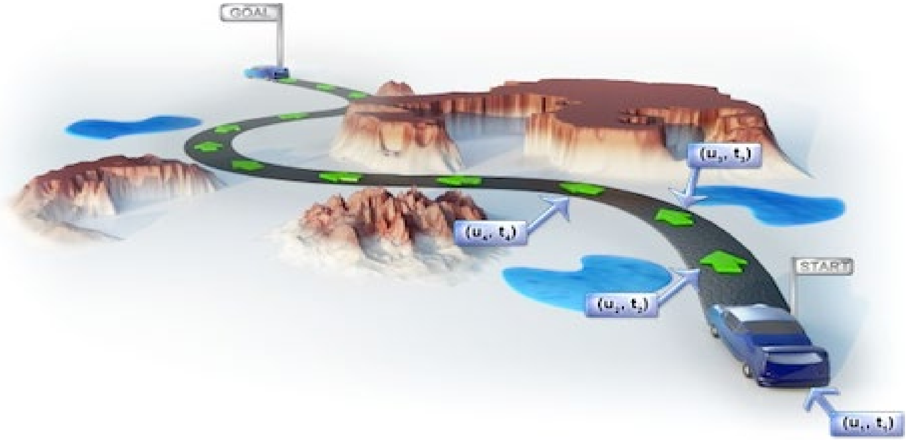
- International undertaking: EU, India, China, S. Korea, Japan, US.
- Goals: Long pulse "burning" plasma. Up to 500 MW fusion power for up to ~1 hr
- Test integrated technology for demonstration reactors
- First plasma aimed for Dec 2025.

Key issue: present-day models too slow for routine full-device experimental prediction and interpretation

Leap from present-day experiments to reactors requires leap in simulation capabilities



Credit © ITER Organization, http://www.iter.org



Reduce costs and risks, by using simulation for:

- Experimental preparation
- Performance optimization
- Model based control
- Reactor design

Computer simulation an important component in fusion reactor design, optimisation, and control

Device prediction from simulation cannot be inferred from isolated behaviour of physics components. Multi-scale, multi-physics problem

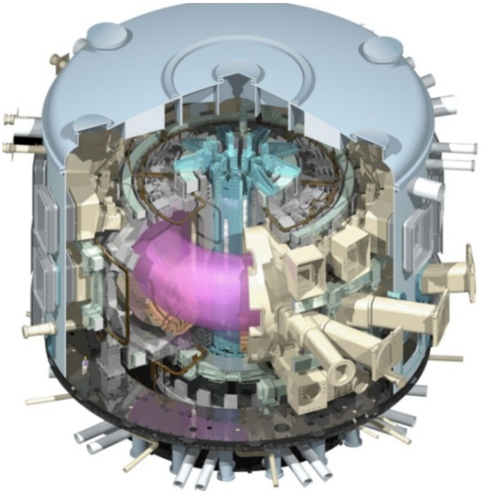
Magnetic equilibrium

Heating

MHD stability

Turbulence

Plasma-wall-interaction



Fusion power

Heat exhaust

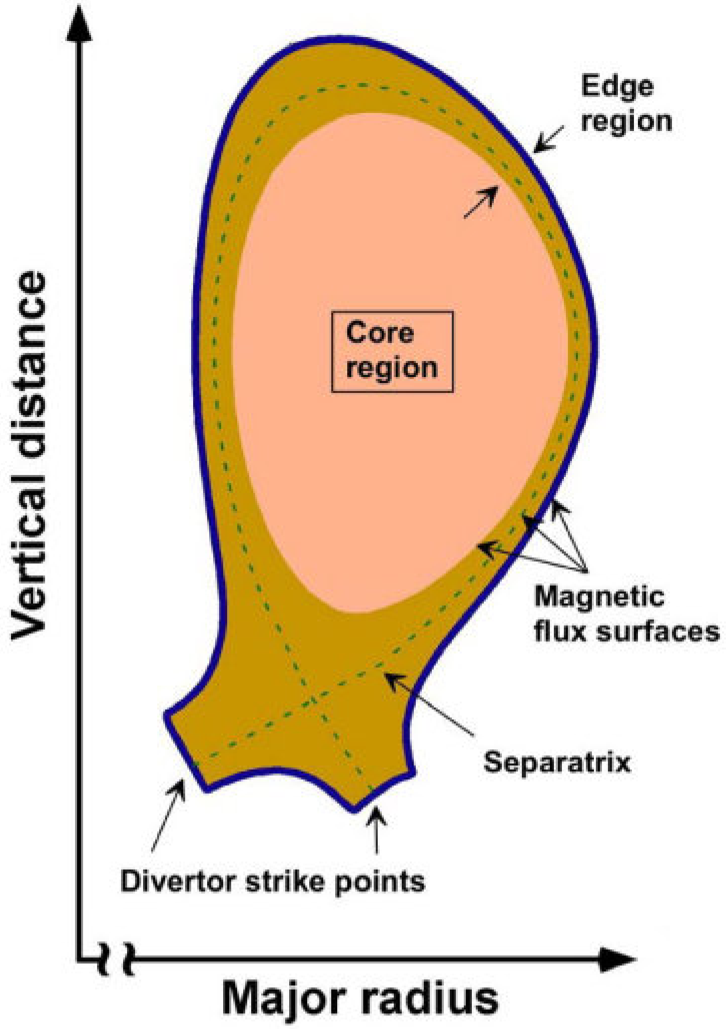
Each physics component demands tractable and accurate models. A multi-fidelity approach is key: capture high-fidelity physics with fast reduced models

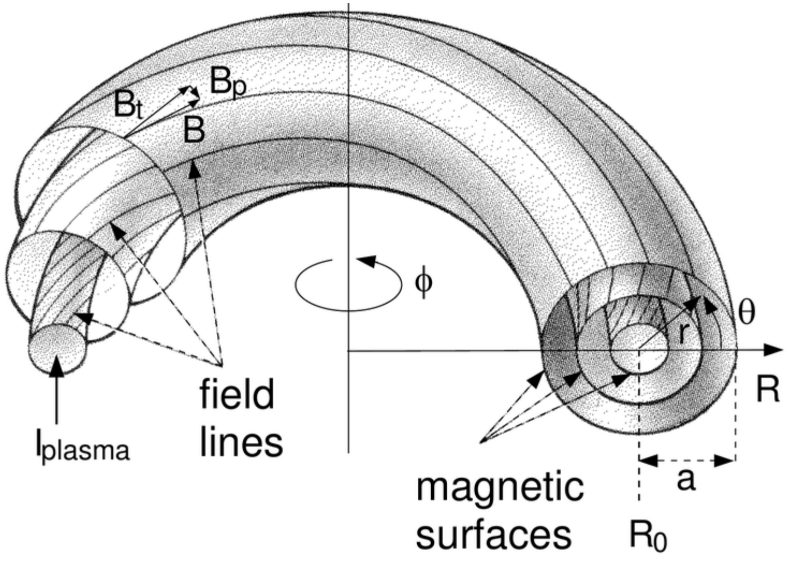
Up next: brief tour of integrated modelling physics components

- Magnetic equilibrium
- Edge and core transport codes
- Plasma heating
- Collisional transport
- Turbulent transport

Disclaimers:
Many components not covered here! MHD, plasma-material-interactions, neutronics, among others…
Will provide flavour rather than in-depth description of computational methods
Focus is on reduced models applicable in integrated modelling, not high-fidelity HPC simulation
Many excellent models and codes exist for all these components, beyond limited examples shown here

Separate plasma regions in core (~1D) and edge (~2D). Different computational challenges that must be integrated

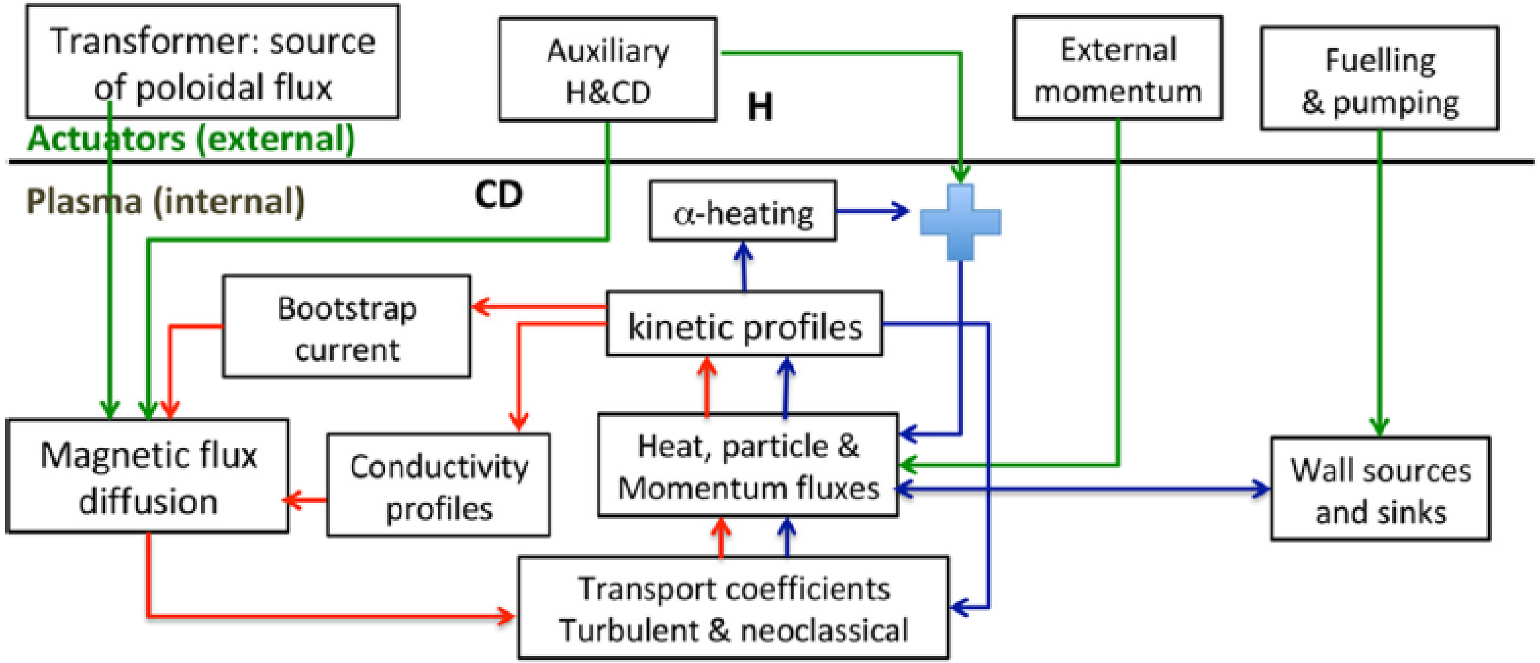




- Core region has nested magnetic surfaces at constant magnetic flux.
- Fast transport along field lines → flux surfaces have constant pressure. Plasma transport (of n, T) is thus radial 1D
- In edge region, magnetic field lines end at wall. Plasma n,T is 2D
- Plasma current, heating, fusion, concentrated in core

Overview of integrated tokamak modelling (multi-physics simulation)

Multiple physics sub-components, multiple nonlinearities



Transformer: source of poloidal flux

Auxiliary H&CD

H

External momentum

Fuelling & pumping

Actuators (external)

Plasma (internal)

CD

α-heating

Bootstrap current

kinetic profiles

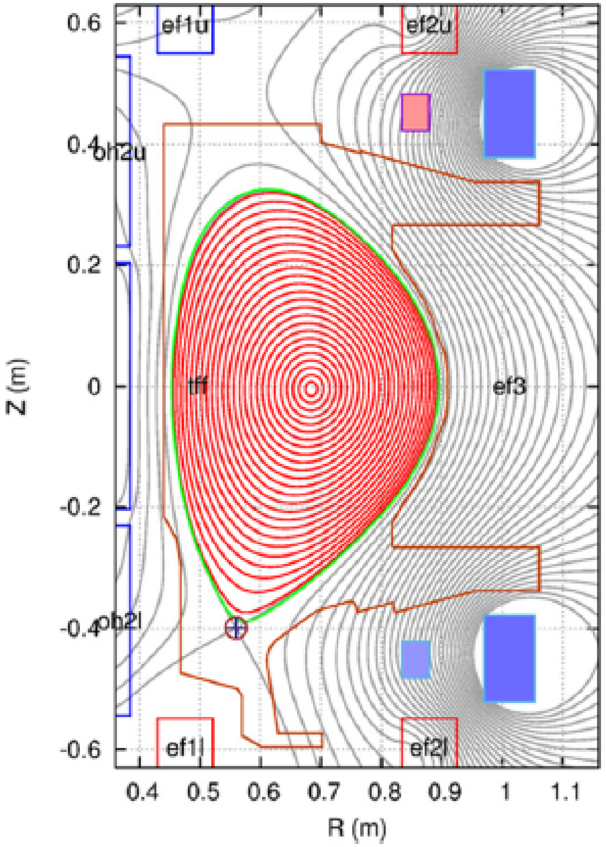
Magnetic flux diffusion

Conductivity profiles

Heat, particle & Momentum fluxes

Wall sources and sinks

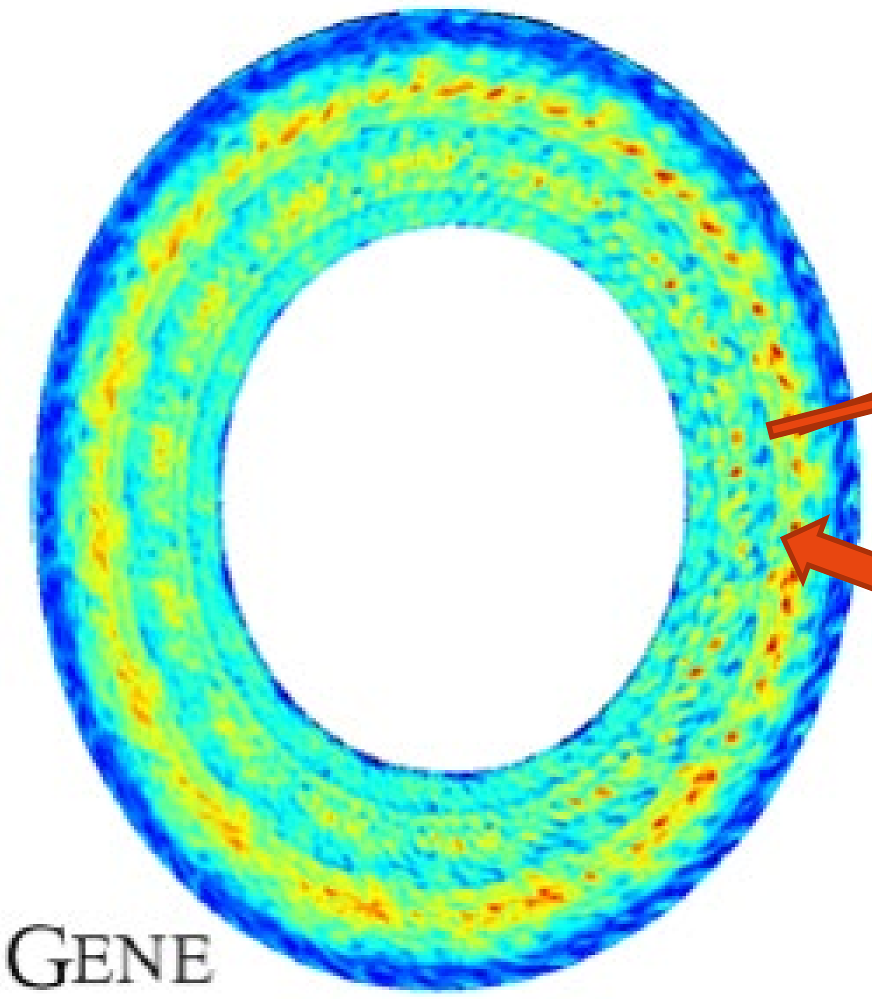
Transport coefficients Turbulent & neoclassical



Kinetic profiles ≡ radial distributions of plasma temperature, density, angular momentum

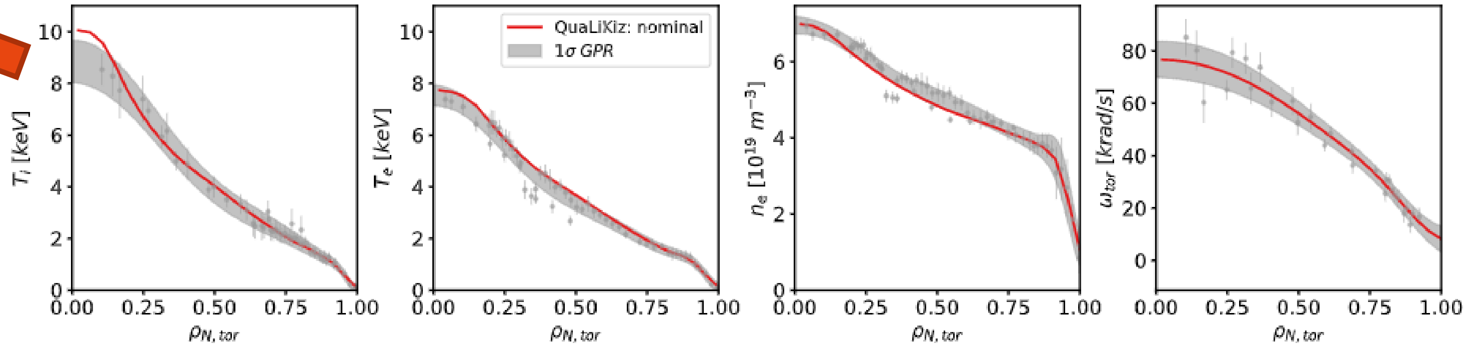
Source: F. Poli Phys. Plasmas 2018 “Integrated Tokamak modeling: When physics informs engineering and research planning”

Necessary innovation: fast models to allow complex system simulations on required timescales to explore new physics



Density,
temperature,
momentum

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \nabla \cdot (\mathbf{v} c) + R$$



QuaLiKiz, reduced gyrokinetic turbulence transport model
[Bourdelle PPCF 2017, Citrin PPCF 2017]

Components of the integrated tokamak simulator: Magnetic equilibrium

$$j \times B = \nabla p$$

$$\nabla \times B = \mu_0 j$$

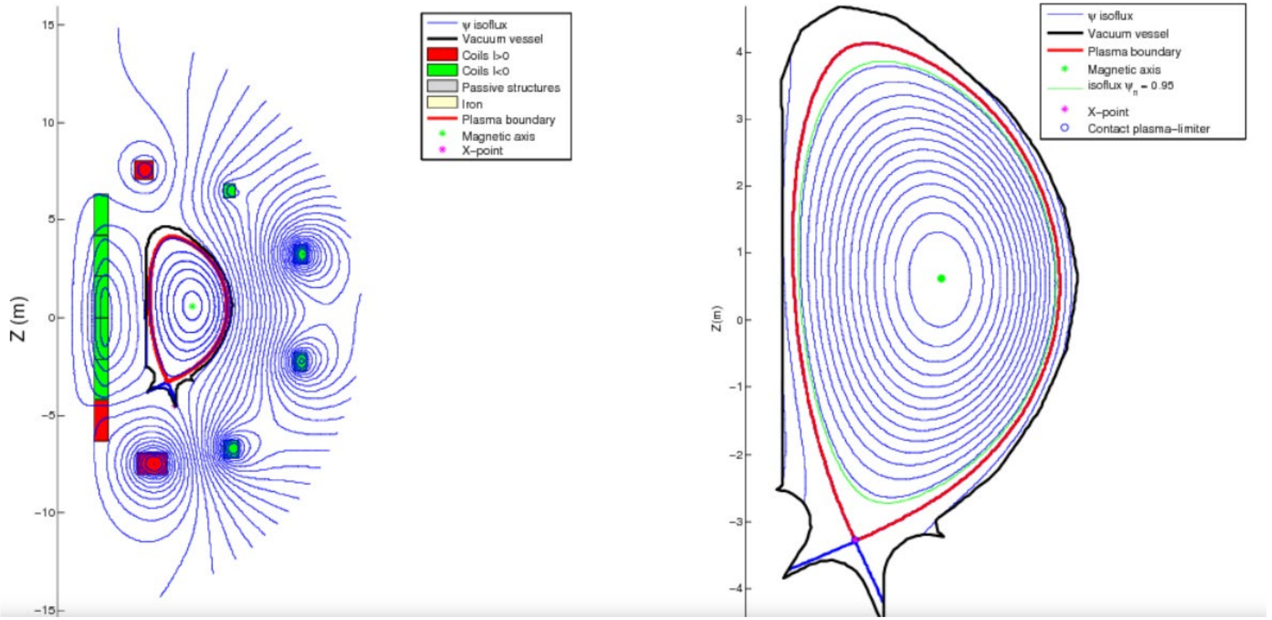
$$\nabla \cdot B = 0$$

Solve force balance equation and magnetostatics (2D PDE with FEM methods). Currents from:

- Active coil circuits
- Induced plasma current
- Induced current in vacuum vessel

Coupled with electromagnetic equations for:

- Diffusion of magnetic field (and current) in plasma
- Evolution of coil currents including mutual inductance

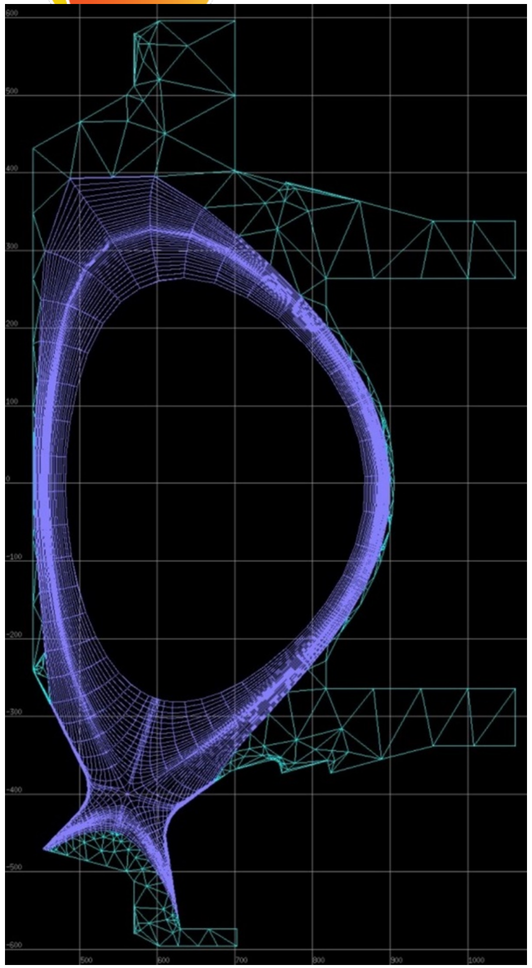


Heumann, Journal of Plasma Physics 2014

Applications

- Designing trajectory of plasma shape, position, and control under constraints (stability, coil limits)
- Define grid for plasma codes in edge and core
- Solve magnetic field distribution in plasma, impacting stability and transport
- Can run in reduced mode for solving core magnetic equilibrium with fixed boundary

Components of the integrated tokamak simulator: Plasma edge modelling

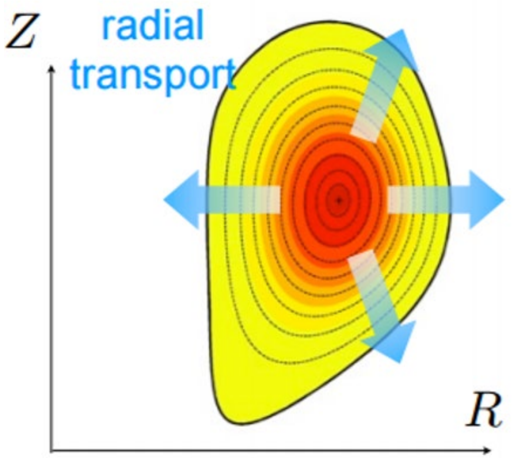


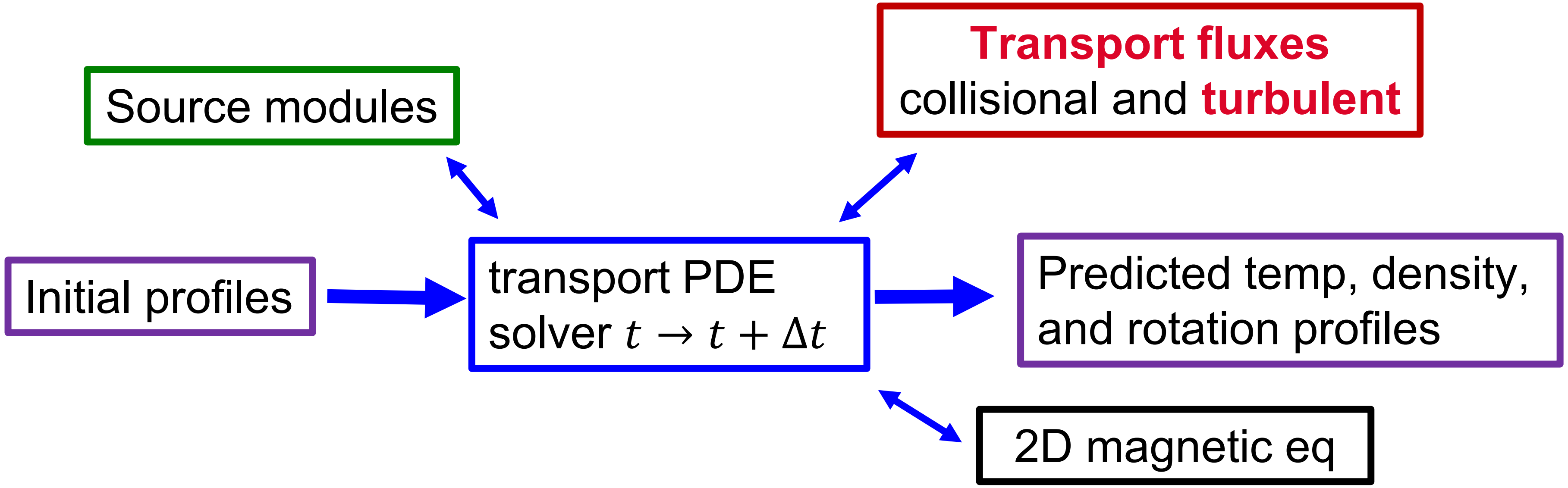
SOLPS-ITER [Wiesen JNM 2015]
EDGE2D-Eirene [Reiter JNM 1992,
Simonini CPP 1994]
UEDGE [Rognlien JNM 1992] … and others!

Vital for assessing fuelling efficiency, impact of plasma exhaust on wall heat loads, heat exhaust mitigation strategies (e.g. impurity seeding).
ITER divertor geometry designed using such simulation suites [Pitts NME 2019]

- Multi-fluid 2D model for ions and electrons
  - ➢ Bragiinski (collisional) closure for conducting fluid model
  - ➢ Cross-field turbulent transport not self-consistently captured. Reduced-order-models of edge turbulence an open research topic!
- 3D kinetic Monte-Carlo model for injected neutrals (e.g. fuelling)
  - ➢ Atomic and molecular interactions with plasma. Particle and energy sources and sinks
  - ➢ Interaction with boundary, e.g. pumping, reflections, absorption.
- Plasma-material-interactions. Monte Carlo neutrals and Molecular Dynamics derived sputtering coefficients, redeposition (e.g. ERO code [Kirschner JNM 07])

Components of the integrated tokamak simulator: Plasma core modelling





Source modules

Transport fluxes
collisional and **turbulent**

Initial profiles

transport PDE solver $t \rightarrow t + \Delta t$

Predicted temp, density, and rotation profiles

2D magnetic eq

Particle flux Particle sources/sinks

Particle density: $$\frac{\partial n_s}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(r\Gamma_s) = S_s$$

Energy: $$\frac{3}{2}\frac{\partial P_s}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(r q_s) = Q_s$$

Heat flux Heat sources/sinks

Typical solver timestep $\Delta t \approx 1ms$. Total simulation ~1-10s (longer for superconducting machines)

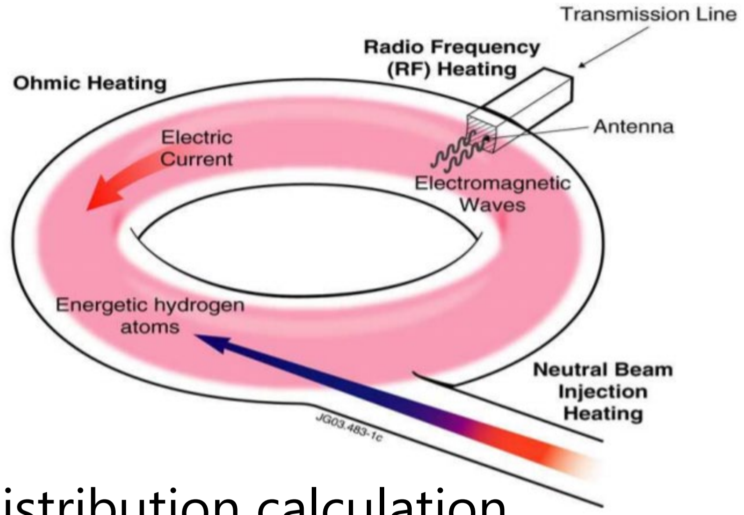
Need for reduced models. e.g. for turbulent transport, nonlinear gyrokinetic simulation costs 10^4 CPUh per call (timestep)

Multiple such modelling frameworks in use, e.g. JINTRAC [1,2], ASTRA [3], ETS [4], TOPICS [5], PTRANSP [6] among others

[1] G. Cenacchi, A. Taroni, JETTO: A free-boundary plasma transport code, JET-IR (1988)
[2] M. Romanelli 2014, Plasma and Fusion research 9, 3403023-3403023
[3] G.V. Pereverzev and Y.P. Yushmanov. ASTRA Automated System for Transport Analysis in a tokamak . IPP - Technical Report, (5/42), 2002
[4] G.L. Falchetto et al 2014 Nucl. Fusion 54 043018
[5] N. Hayashi et al 2010 Phys. Plasmas 17 056112
[6] R.V. Budny 2009 Nucl. Fusion 49 085008

Components of the integrated tokamak simulator: Heating and current drive

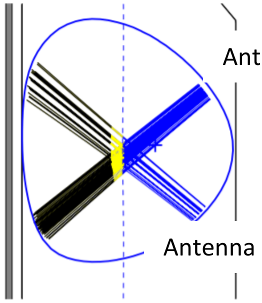
Multiple methods of plasma heating. Among most common are:
Ion Cyclotron Resonance Heating (ICRH)
Electron Cyclotron Resonance Heating (ECRH)
Neutral Beam Injection (NBI)



EM-wave calculations

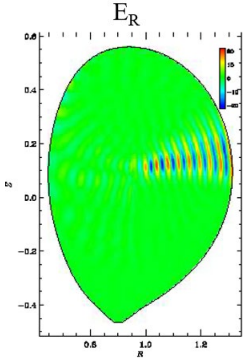
$$\nabla \times \nabla \times \vec{E} = \frac{\omega^2}{c^2}\overleftrightarrow{\epsilon}(f_i)\cdot\vec{E} + i\omega\mu_0\vec{j}_{ext}$$

Plasma Dielectric tensor $\bar{\epsilon}$ from kinetic theory
j_{ext} ≡ antenna curent



Coda IAEA FEC 2008

ECRH – ray tracing (mm waves) in plasma medium and absorption by electrons at resonant frequency overview: Prater NF 2008



Eriksson NF ‘93

ICRH – full wave solver (direct solution of Maxwell equations)
e.g. TORIC [Brambilla PPCF 1999]

Velocity distribution calculation

NBI: ionization of accelerated neutral beam and collisional heating of plasma. Asymmetry → driven plasma current

ICRH: Resonant ion excitation by wave + collisions (heating)

Two main methods
- Monte Carlo – follow ion trajectories and average
- Fokker-Planck - solve equation for distribution function

Components of the integrated tokamak simulator: Collisional (neoclassical) transport

Drift kinetic equation

$$\frac{\partial f_a}{\partial t} + (v_\parallel \mathbf{b} + \mathbf{v}_{da}) \cdot \nabla f_a = C_a(f_a)$$

Parallel (to B-field) streaming

Perpindicular drifts due to e.g. field inhomogenity (ordered lower than $v_\parallel$)

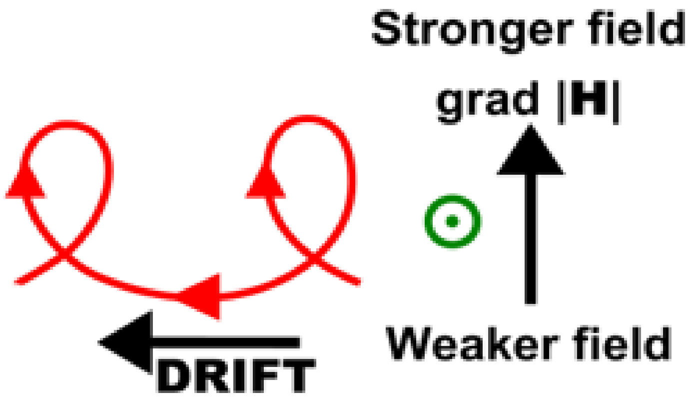
Collision operator

Static solution and perturbation around f_0 Maxwellian

$$v_\parallel \nabla_\parallel f_{a0} = C_a(f_{a0}),$$

$$v_\parallel \nabla_\parallel f_{a1} + \mathbf{v}_{da} \cdot \nabla f_{a0} = C_a(f_{a1})$$

Solve for f_{a1}. Complex due to collision operator form.
Note: radial gradients in T,n, drive f_1 perturbation



- Heat and particle transport from moments of f_1. Impurity particle transport can be significant (large collisionality)
- Plasma current $\sum Z_a \int v_a f_{a1} dv$ arises through perpindicular drifts and collisions. “Bootstrap Current”. Reduces need for external current drive, good for tokamak efficiency
- Popular neoclassical codes: NEO [Belli PoP 2008], NCLASS [Houlberg PoP 1997]

Helander and Sigmar “Collisional Transport in magnetized plasmas” 2005 Cambridge University Press

Gyrokinetic model of plasma turbulence

Kinetic approach: fundamental object is distribution function $f(\boldsymbol{x}, \boldsymbol{v})$

$$n = \int f d^3 v$$
$$\boldsymbol{u} = \int \boldsymbol{v} f d^3 v$$
$$T \propto \int v^2 f d^3 v$$

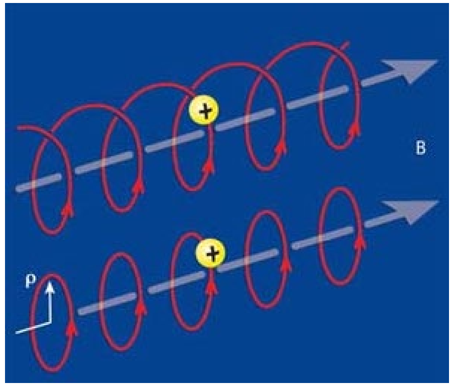
Vlasov equation: Liouville theorm $\frac{df}{dt} = 0$

$$\left[\frac{\partial}{\partial t} + \boldsymbol{v} \cdot \frac{\partial}{\partial \boldsymbol{x}} + \frac{q_j}{m_j}\left(\boldsymbol{E} + \frac{\boldsymbol{v}}{c} \times \boldsymbol{B}\right) \cdot \frac{\partial}{\partial \boldsymbol{v}}\right] f_{j(\boldsymbol{x}, \boldsymbol{v}, t)} = 0$$

Leads to nonlinearity
(self-generated fields)

Field equations

$$\begin{aligned} \nabla \times E &= -\frac{1}{c}\frac{\partial B}{\partial t} \\ \nabla \times B &= \frac{4\pi}{c}\sum_j q_j \int v f_j \mathrm{d}v + \frac{1}{c}\frac{\partial E}{\partial t} \\ \nabla \cdot E &= 4\pi \sum_j q_j \int f_j \mathrm{d}v \end{aligned}$$



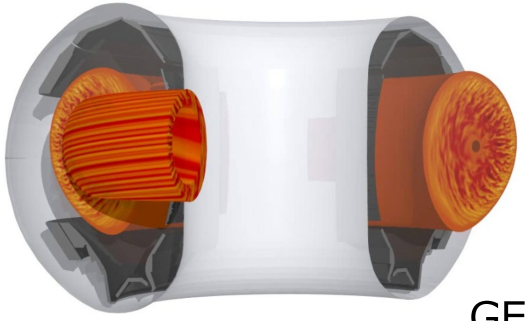
(Plot from SCIDAC review 2005)

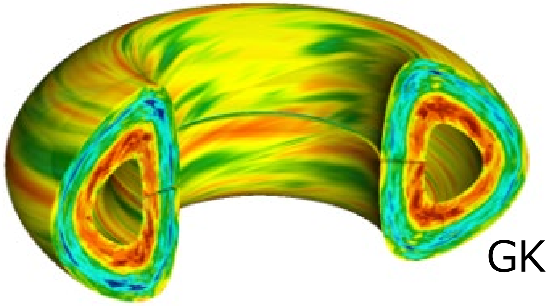
- Major computational speedup by averaging over fast gyromotion around field lines. 6D→5D, larger timesteps
- Justified since instability frequency (10-100 kHz) much lower than gyrofrequency (10-100 MHz for ions)
- Kinetic theory of charged particle rings → “gyrokinetics”

Multiple groups and codes worldwide working on simulations and interpretation of gyrokinetic turbulence and comparison with experiment

Direct numerical simulation codes for nonlinear tokamak turbulence, e.g.

GENE (www.genecode.org)
GKW (http://www.gkw.org.uk)


GENE

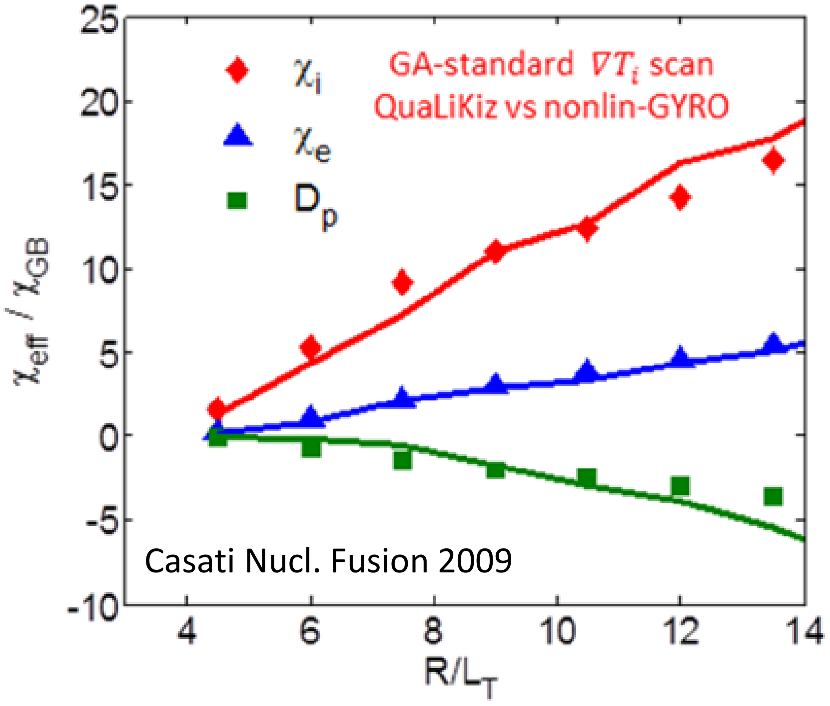

GKW

Theory breakthroughs and high-performance-supercomputing led to amazing advances in past 20 years
Quantitative agreement with experiments across multiple regimes – active area of research

But… simulations too expensive and slow for routine use for modelling and optimization of tokamak scenarios. $10^4 - 10^6$ CPUh for each evaluation!

Significant speedup of turbulence simulation by reduced (quasilinear) order models

Quasilinear vs nonlinear heat convection and particle diffusion comparison



Casati Nucl. Fusion 2009

- Weak turbulence assumption (justified by analysing nonlinear simulations). Turbulent transport dominated by fluctuations that maintain linear instability characteristics. Nonlinear physics sets amplitude level.

- Two-part model:
  - Solve (simplified) linear gyrokinetic dispersion relation
  - Set mode saturation based on a model based on analytical considerations, turbulence measurements and nonlinear simulations

- 10 CPU seconds to calculate fluxes at a single radial point. $\times 10^6$ faster than nonlinear

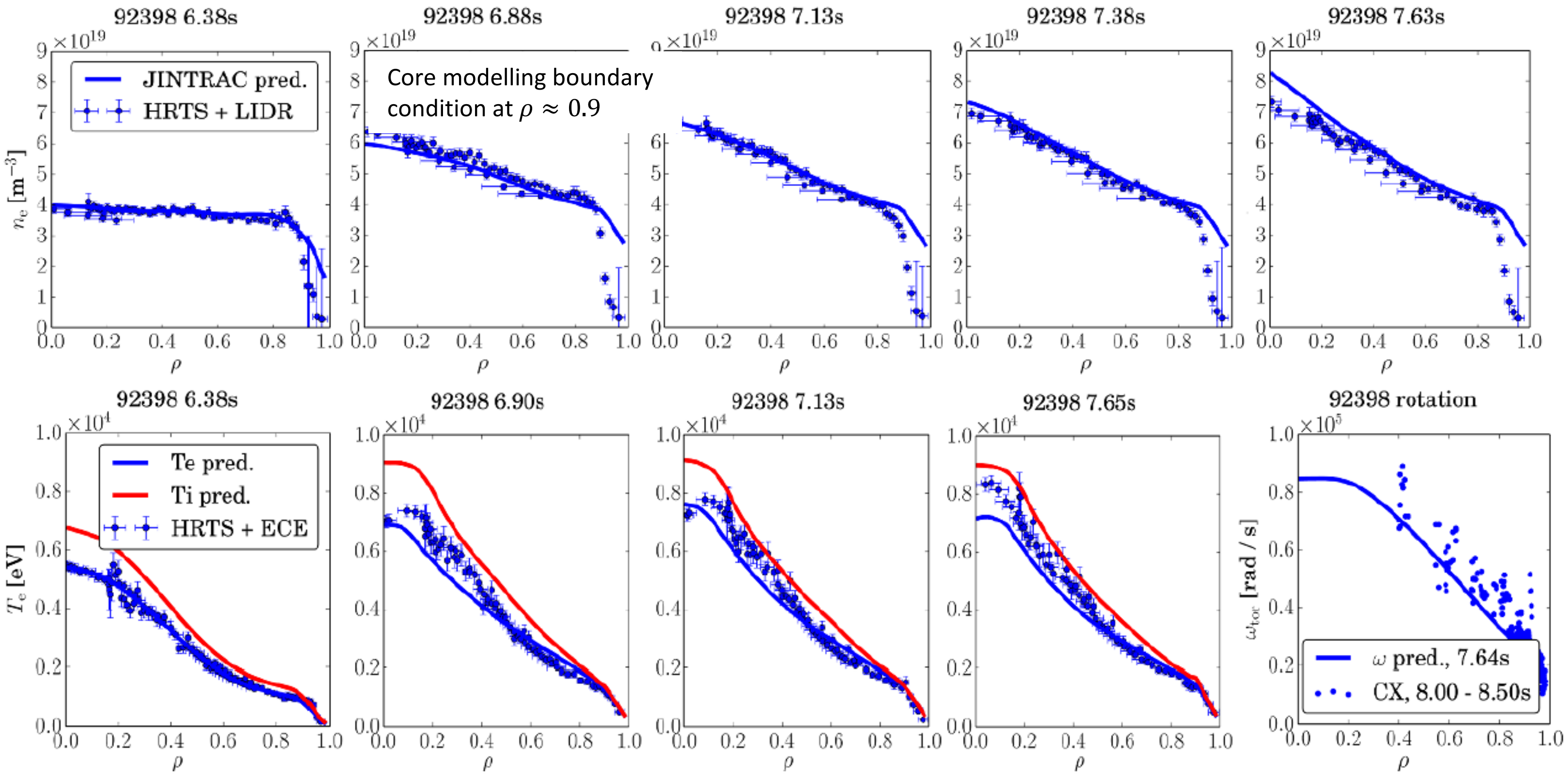
- Allows tokamak discharge evolution simulation in reasonable time: ~several days on single node in cluster

Examples:
TGLF [Staebler PoP 2007]
QuaLiKiz [Bourdelle PPCF 2016, Citrin PPCF 2017, Stephens JPP 2021, www.qualikiz.com]

Up next: case studies

- Integrated modelling application at JET: modelling of impurity W plasma penetration
- Development of a fast and accurate turbulence transport modelling with neural networks

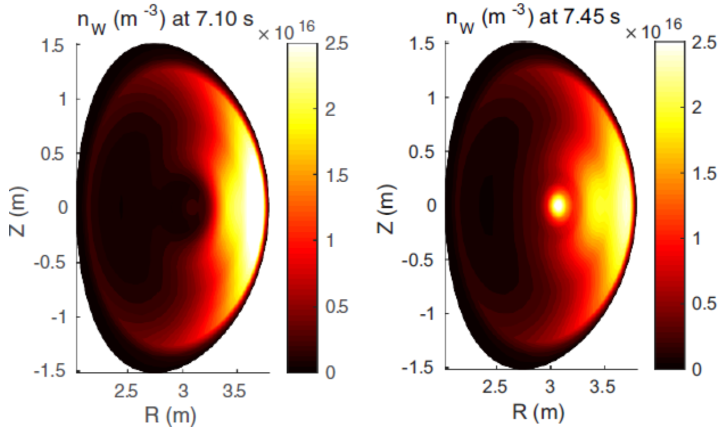
Example application: W-accumulation at JET tokamak due to density peaking, and avoidance with ICRH



Core modelling boundary condition at $\rho \approx 0.9$

W-radiation emission peaks at later time due to inward neoclassical W transport driven by density peaking.

Mitigated by on-axis ICRH heating (not shown for brevity)



JINTRAC-QuaLiKiz-NEO successfully described core W-accumulation in JET and mitigation strategy with ICRH heating [Casson NF 2020, Breton NF 2018].

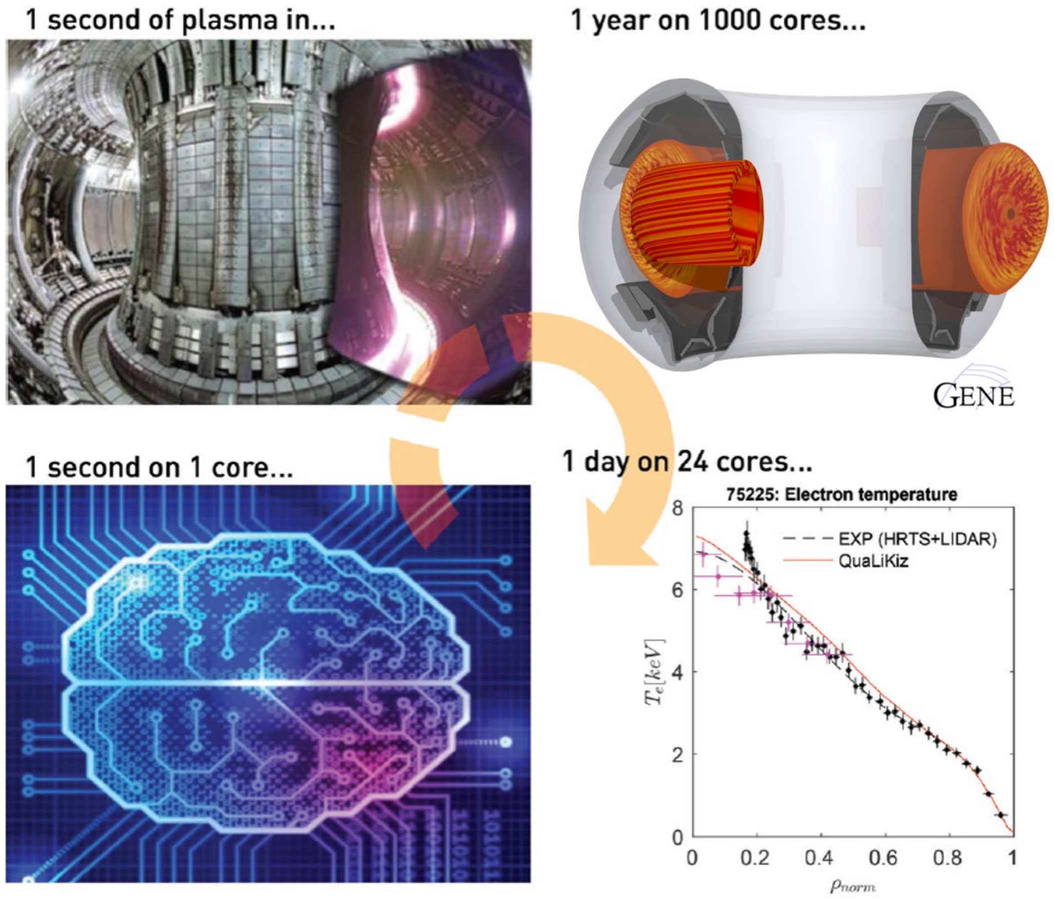
State-of-the-art core plasma integrated modelling. Combined evolution of temperatures, densities, rotation, impurities for the first time. Non-trivial interactions between turbulence (sets main profiles), neoclassical transport (sets W transport), heating

Neural networks learn the reduced turbulence model directly and replace it in tokamak simulation

$10\ CPUs$ per flux is fast, but we can go much further!

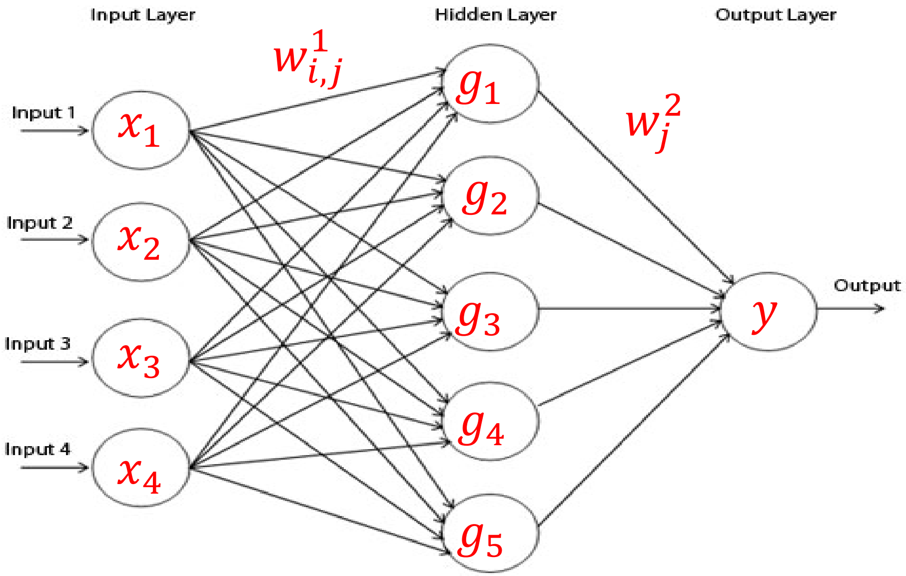
1. Quasilinear model tuned to nonlinear simulations and validated against experiments
2. Use to generate large datasets of turbulent calculations in relevant tokamak parameters
3. Feed-forward neutral networks for regression of the model multivariate input-output map
4. Use the trained NN as a surrogate transport model for tokamak simulation. Evaluating the trained NN is ~5 orders of magnitude faster than QuaLiKiz!

   1 trillion times faster than the anchoring nonlinear simulations



Neural network regression of QuaLiKiz dataset has relatively low input dimensionality. Sufficient to apply “simple” fully connected FFNN

Fully connected feedforward neural network (simple topology)



x: Inputs, e.g. temperature and density gradients,
magnetic geometry info
y: Output: e.g. ion heat flux
w: free weights for optimization

$$y = \sum w_j^2 g_j \left(\sum w_{i,j}^1 x_i \right)$$

With, e.g. $g(x) = \tanh(x)$

Optimize weights by minimizing cost function: $C = \sum_N (t_N - y_N)^2 + \lambda \sum \left(w_{ij}\right)^2$

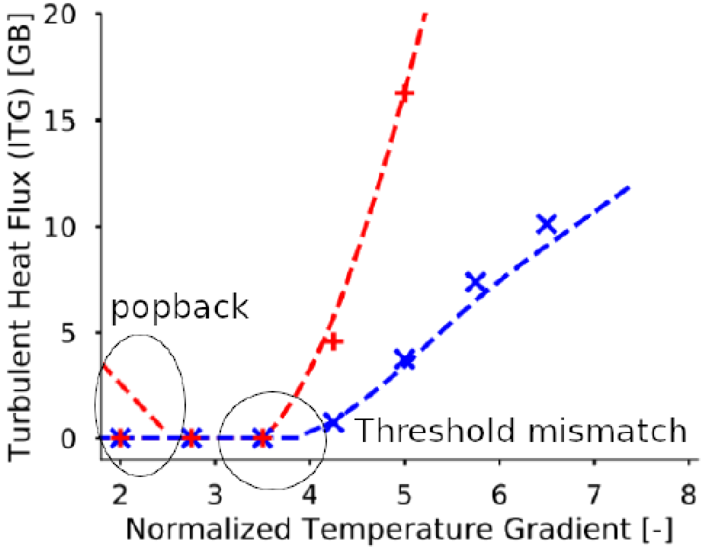
t_N are target values from generated dataset
λ is the regularization factor. Critical for avoiding overfitting

Additional advantage: provides an analytical formula with analytical derivatives. Turbulent flux derivatives with respect to inputs important for implicit timestep PDE solvers and trajectory optimization

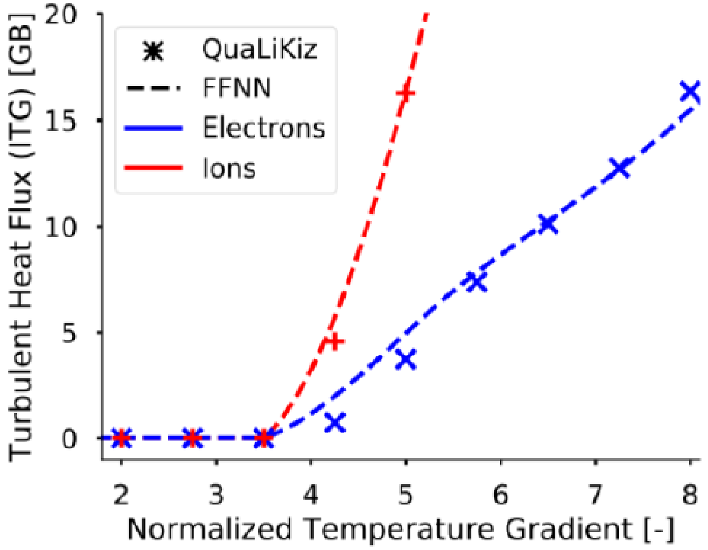
Key point is that RMS error is not a sufficient metric to determine quality of neural network fit. Emply prior knowledge of system!

Incorporate physics-knowledge into NN training. Tokamak turbulent transport has sharp “critical threshold” behaviour

- Global statistics (RMS) less important than local (threshold)
- Same threshold for all transport channels essential
- Achieved by customising training targets and optimisation cost function with physics constraints



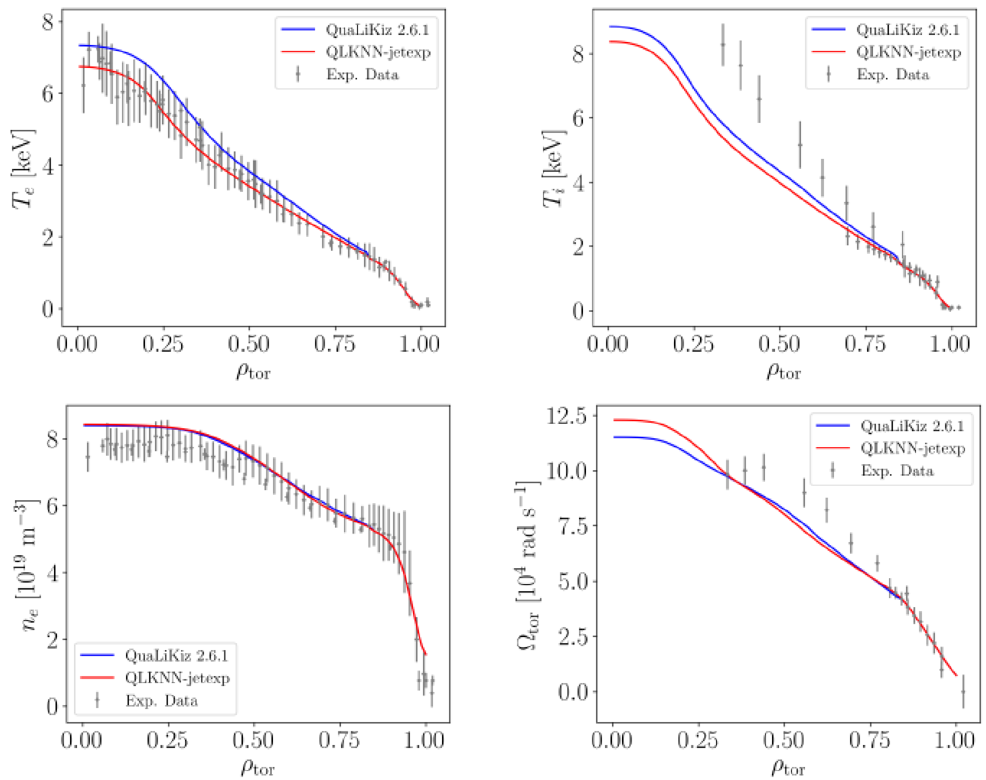
Bad fit



Good fit

Case study: NN for turbulence surrogate model

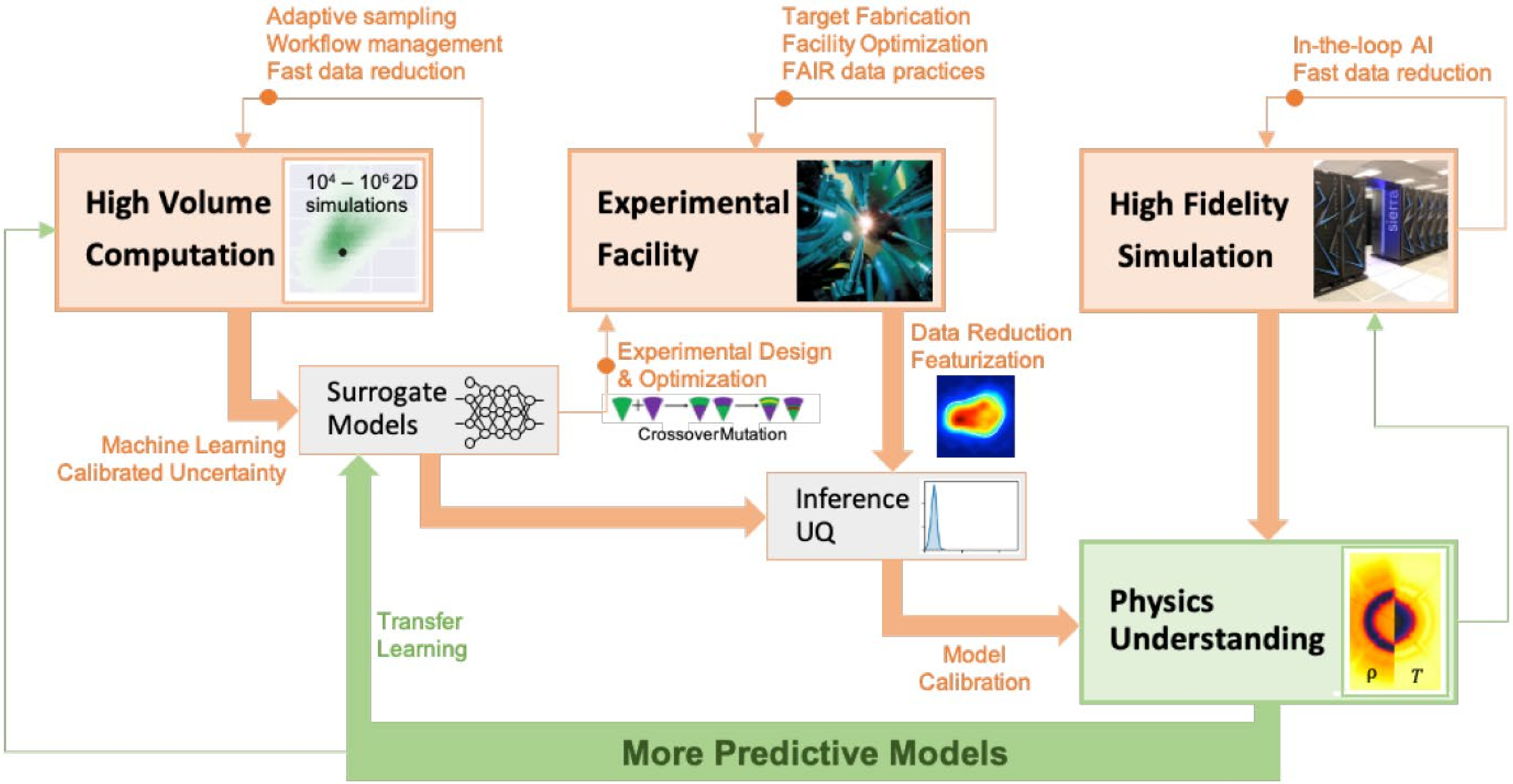
JET baseline #92436



- Training set for QuaLiKiz neural network sampled from multiple time windows from 2145 JET discharges (based on JETPEAK)
- Training set varied T, n, v_{tor} gradients based on error bars of Gaussian Process Regression fits [Ho NF 2019].
  $\sim 20M$ I/O sets
- NN model trained and validated against full-QuaLiKiz and range of JET experiments in multiple regimes
- Currently being applied for JET scenario rampup optimization for T and DT campaigns
- Fast! JINTRAC-QuaLiKiz: ~3 days on 16 cores
  QuaLiKiz-neural-network: ~2 hours on 1 core
  (and turbulent transport no longer in integrated model)

K.L. van de Plassche PoP 2020, A. Ho PoP 2021

Looking ahead: integrating information sources towards fast and accurate modelling for experimental design



Hatfield Nature Perspectives 2021 (focus on Inertial Confinement Fusion, but highly relevant also for Magnetic Confinement Fusion)

Summary

- Integrated tokamak modelling – highly complex coupling of multiple physics components across spatiotemporal scales

- Need for speed: high-fidelity first-principle simulations too slow for integrated modelling with many-query applications. Focus on reduced-order-models

- Much predictive success and experimental design achieved already with integrated modelling. But many sub-components still not fast or accurate enough. Ongoing work

- Surrogate modelling with machine learning a highly promising acceleration path

- Must be coupled with improvements in data inference, simulation validation workflows, tools for experimental design and optimization