



DIFFER

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



EUROfusion

JET



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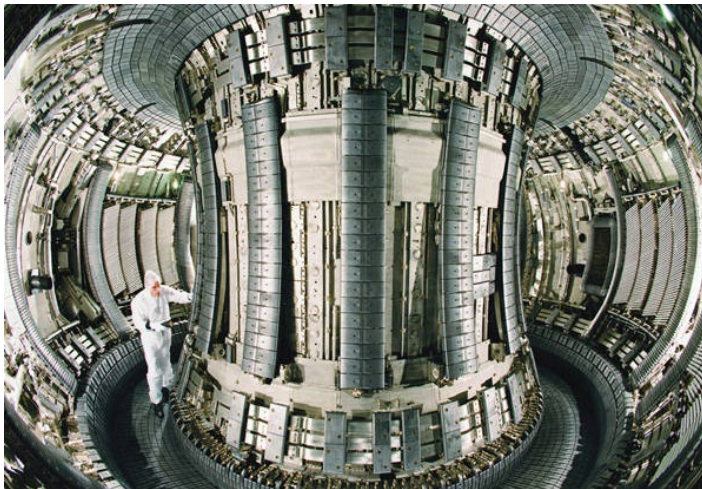
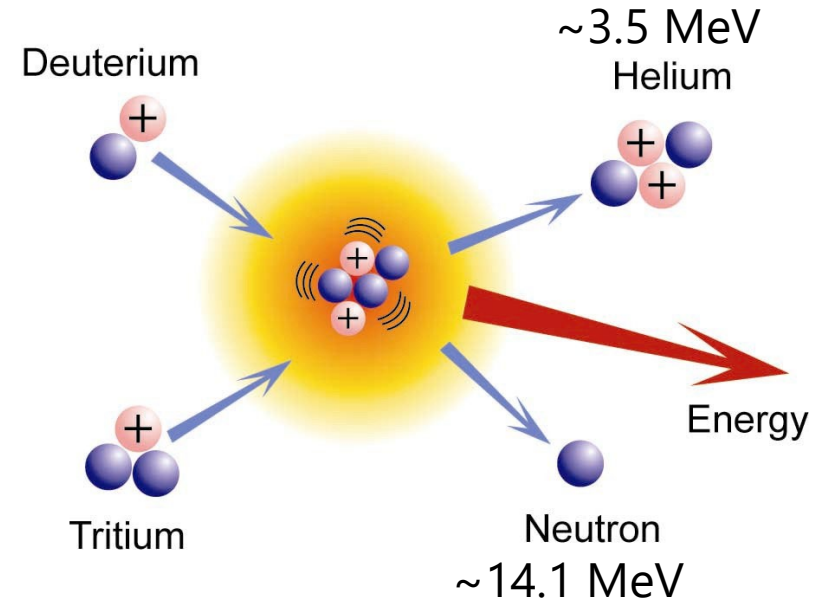
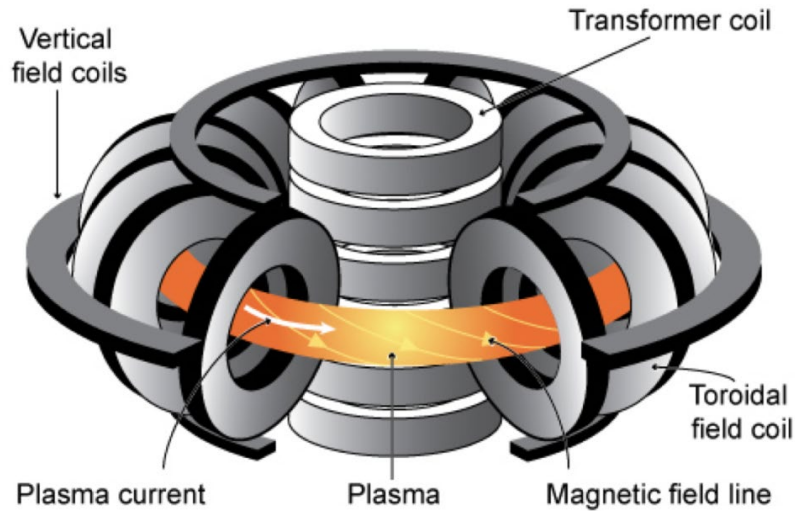


Short Bio

- 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



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

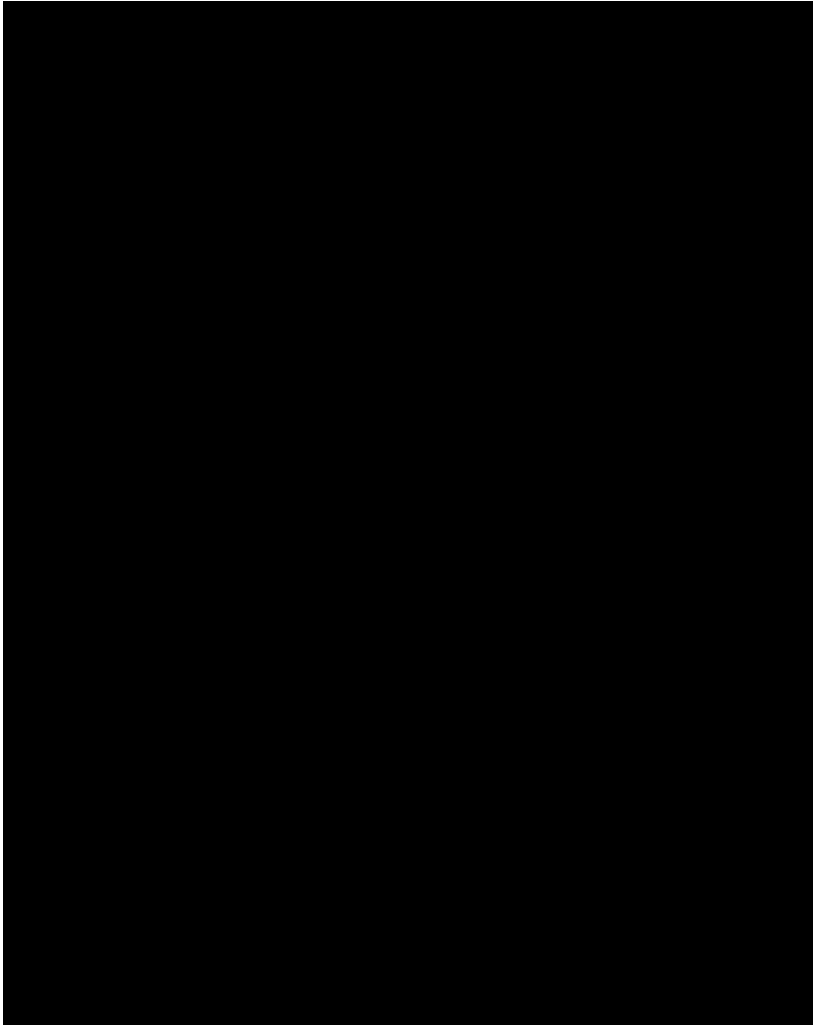


Joint European Torus (JET) - UK

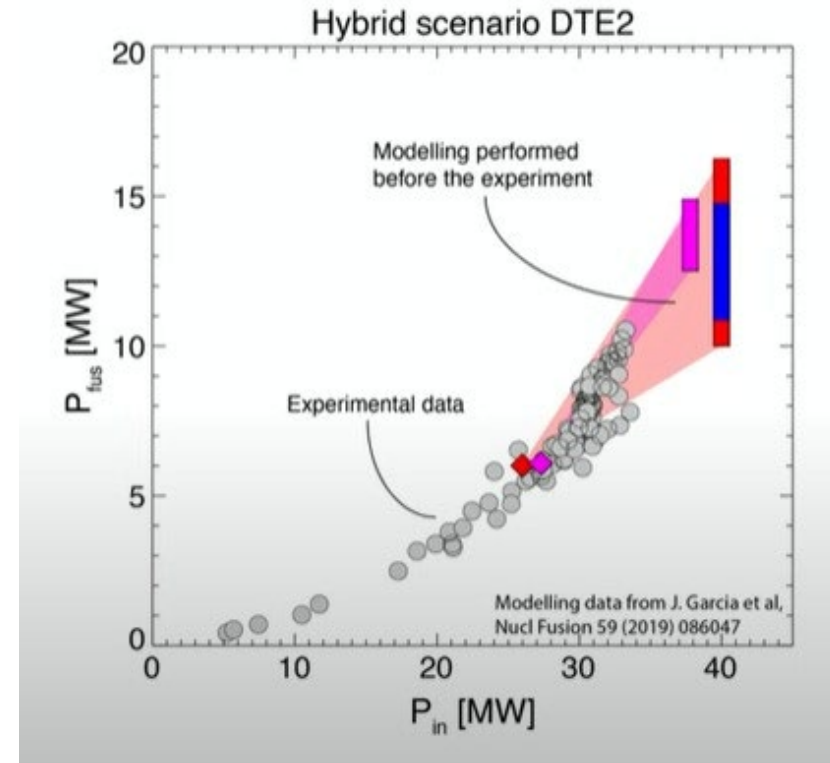
- Helical magnetic field needed to achieve confinement
- Typical parameters: $R = 2$ m, $B = 5$ T, $T = 20$ keV ($\sim 10^8$ K), $n = 10^{20}$ m⁻³
- Heated to fusion conditions by radiofrequency waves and accelerated beams
- Plasma confinement limited by instabilities and turbulence



Exciting times in fusion science



(no movie in PDF version)



World record fusion energy at the JET tokamak 12.21.2021

- ~11MW fusion power for ~5 secs (copper coil limit)
- Multiphysics modelling correctly predicted fusion power in experiments
- With ITER-like-wall. Provides confidence for next step

Next generation of experiments to achieve net fusion gain for first time - last stage before demo reactors

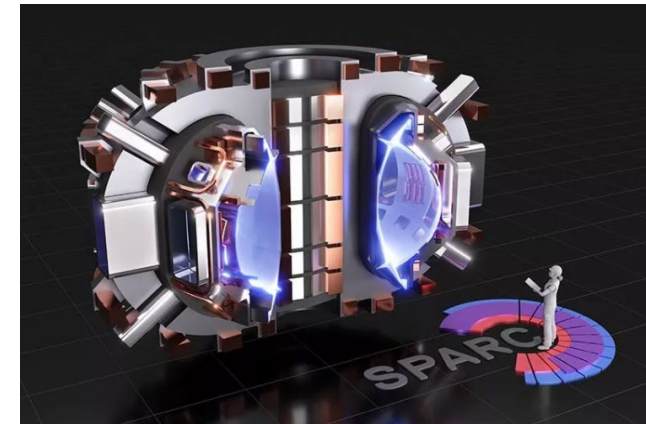


ITER construction in Cadarache, France



- International ITER project. First plasma goal for 2025. 500 MW fusion power
- Advances in high field superconducting (HFS) magnets - parallel exciting developments

SPARC HFS tokamak. First plasma goal 2025



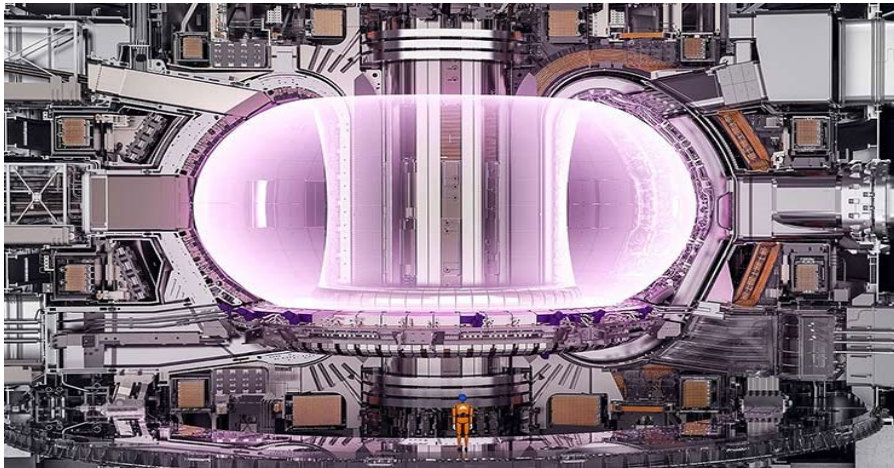
Credit © ITER Organization, <http://www.iter.org>

MIT/Commonwealth Fusion Systems (start-up)



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

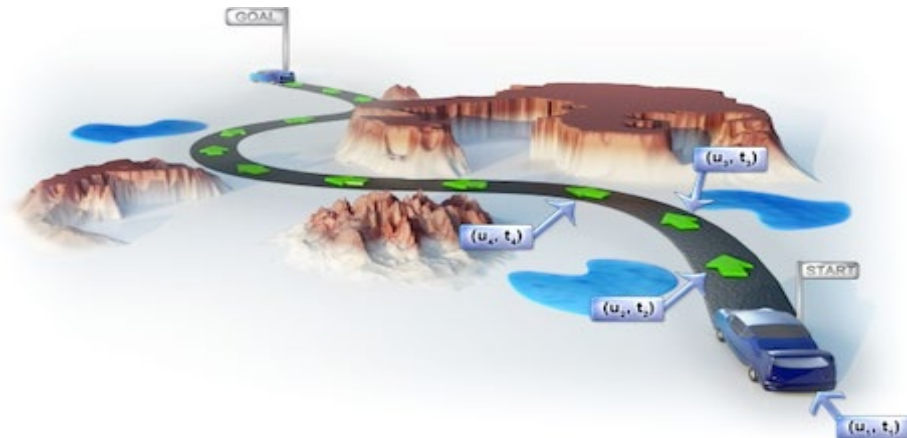
Leap from present-day experiments to reactors requires leap in simulation capabilities



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



Magnetic equilibrium

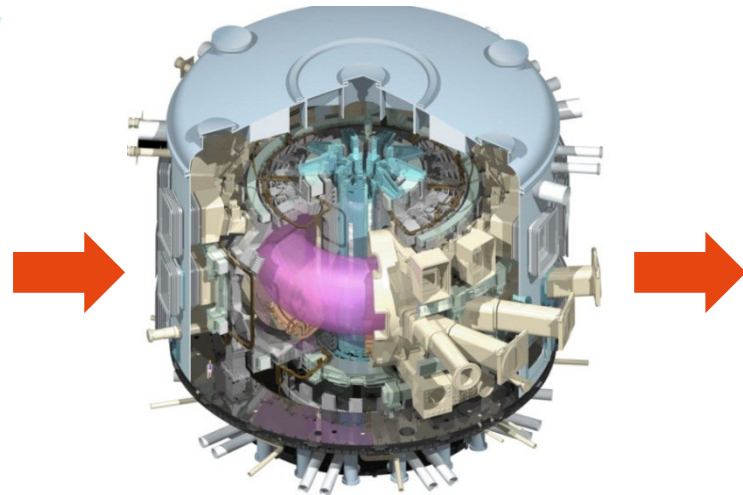
Heating

MHD stability

Turbulence

Plasma-wall-interaction

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



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

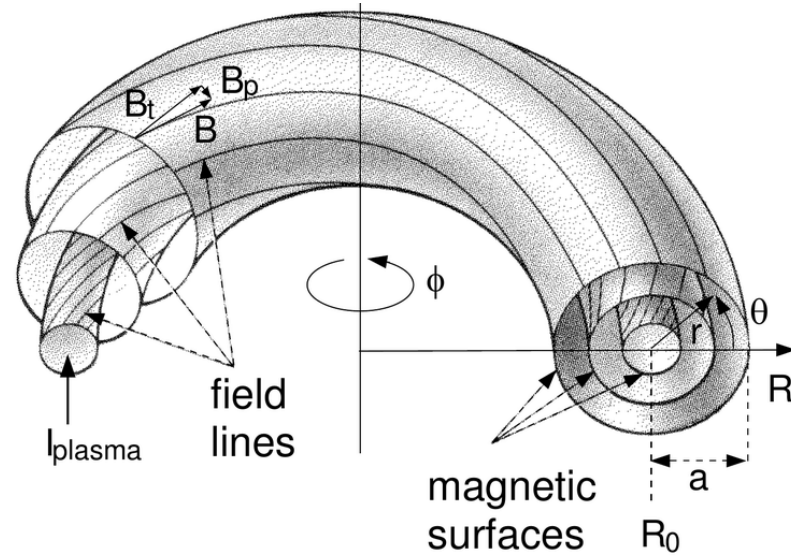
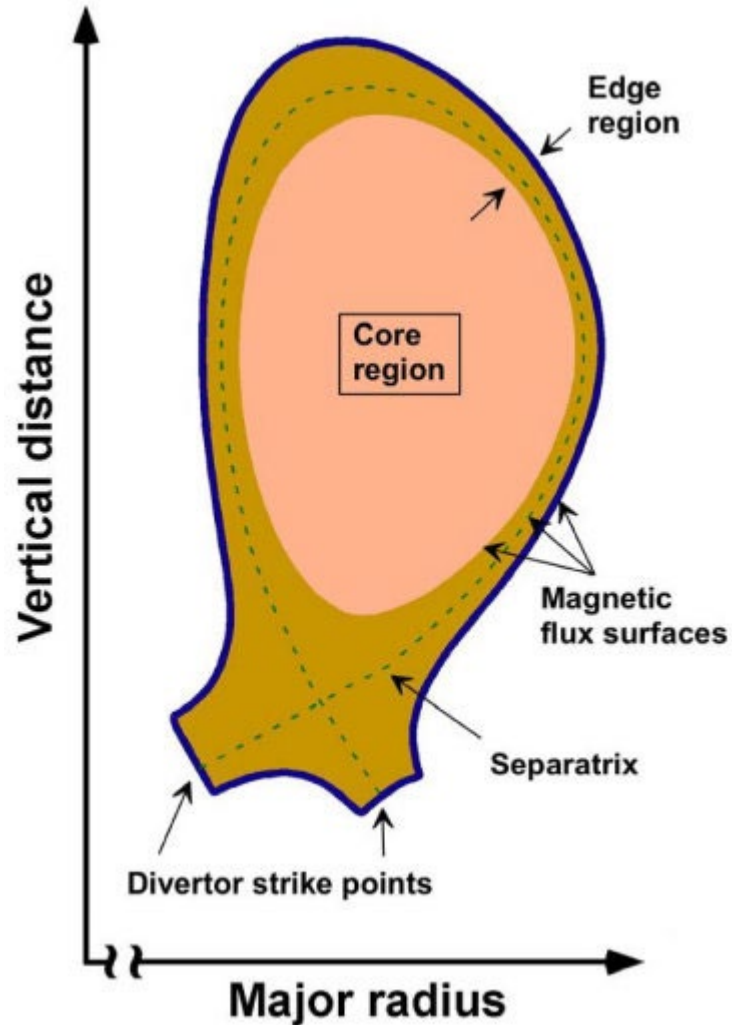
- Edge and core transport codes
- Modelling use-cases
- Physics components (subset)
 - Magnetic equilibrium
 - Plasma heating
 - Collisional and turbulent transport

Disclaimers:

Many components not covered here! MHD, plasma-material-interactions, neutronics, among others...
Will provide flavour rather than in-depth description of computational methods

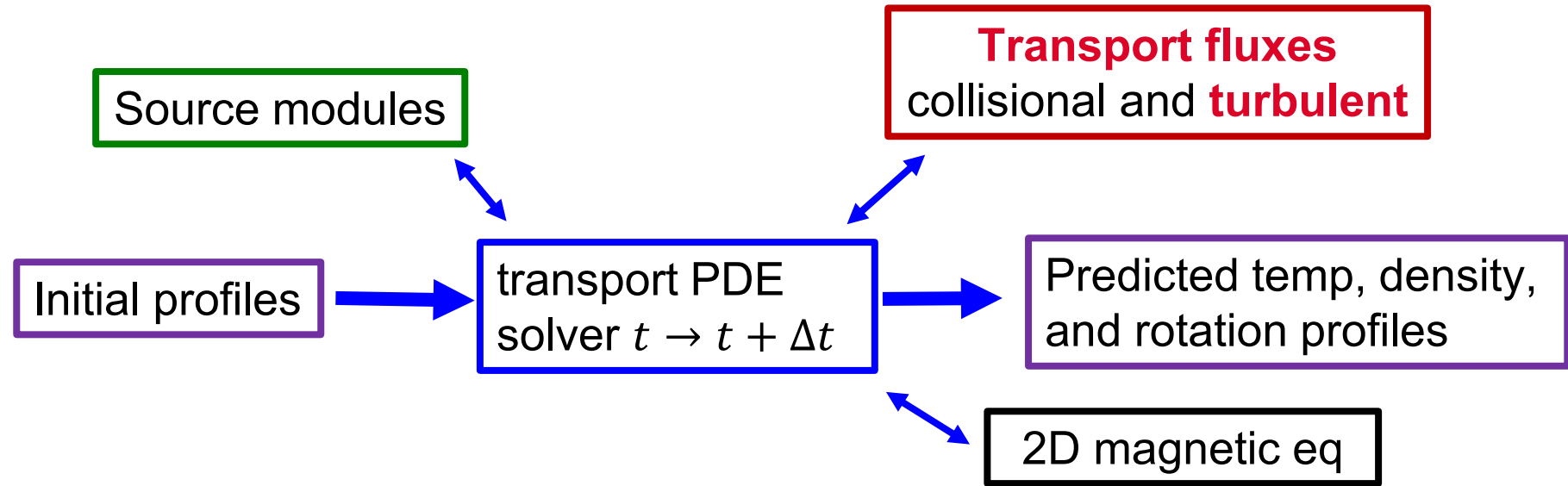
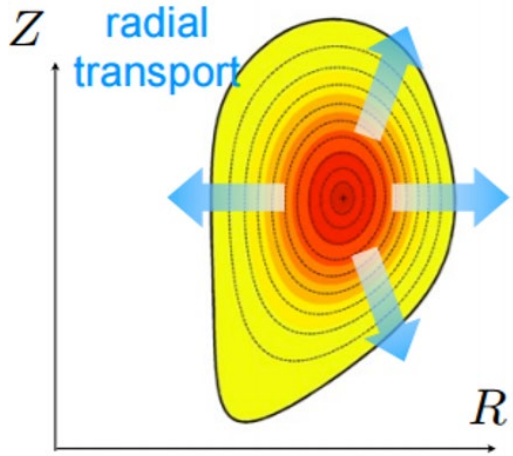
Focus is on reduced order models applicable in integrated modelling, not high-fidelity HPC simulation
Many excellent models and codes exist for all these components, beyond limited examples shown here

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



- Core region has nested magnetic surfaces at constant magnetic flux.
- Fast transport along field lines \rightarrow 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, more complex transport description
- Plasma current, heating, fusion, concentrated in core

Components of the integrated tokamak simulator: Plasma core modelling



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

Labels: Particle flux (points to $r \Gamma_s$), Particle sources/sinks (points to S_s)

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

Labels: Heat flux (points to $r q_s$), Heat sources/sinks (points to Q_s)

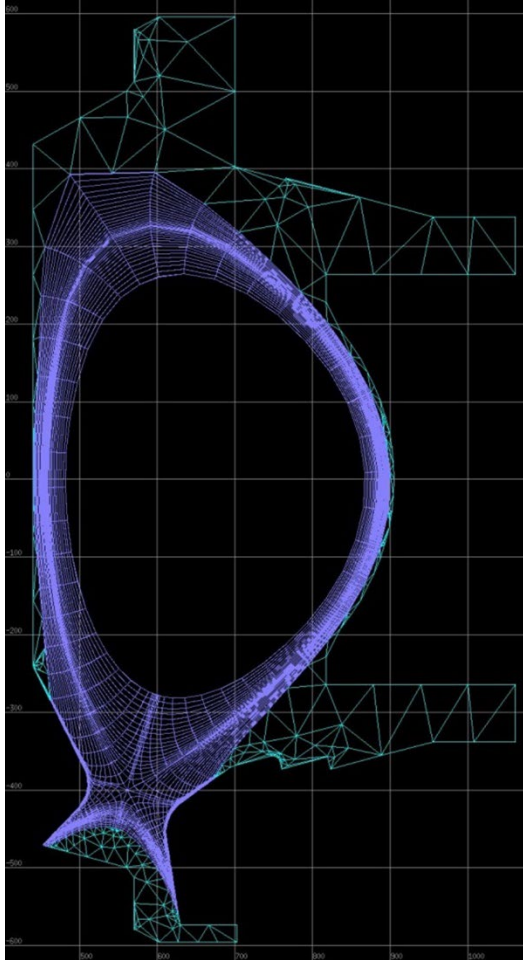
Typical solver timestep $\Delta t \approx 1ms$. Total simulation $\sim 1-10s$
(longer for superconducting machines)

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: Plasma edge modelling



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 for particle and energy sources/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])

SOLPS-ITER [Wiesen JNM 2015]

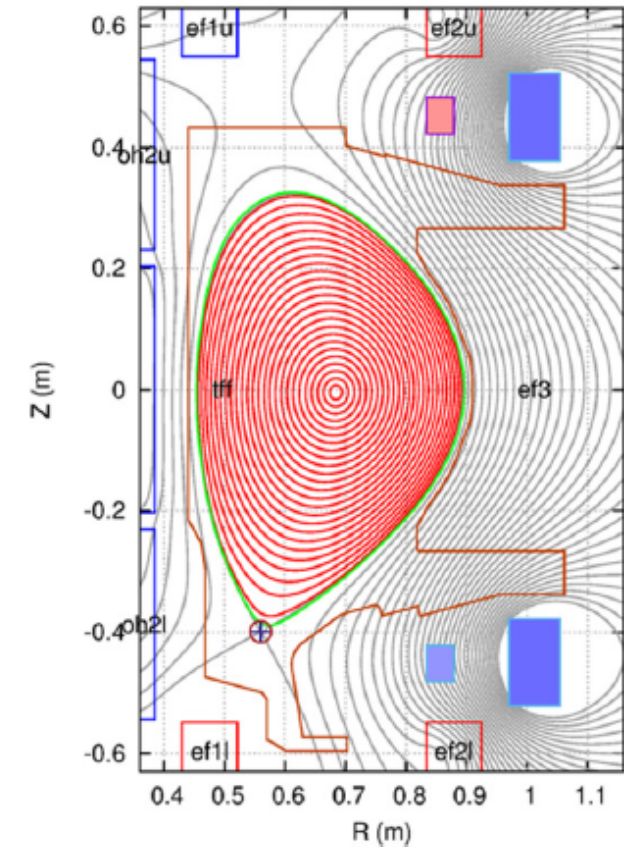
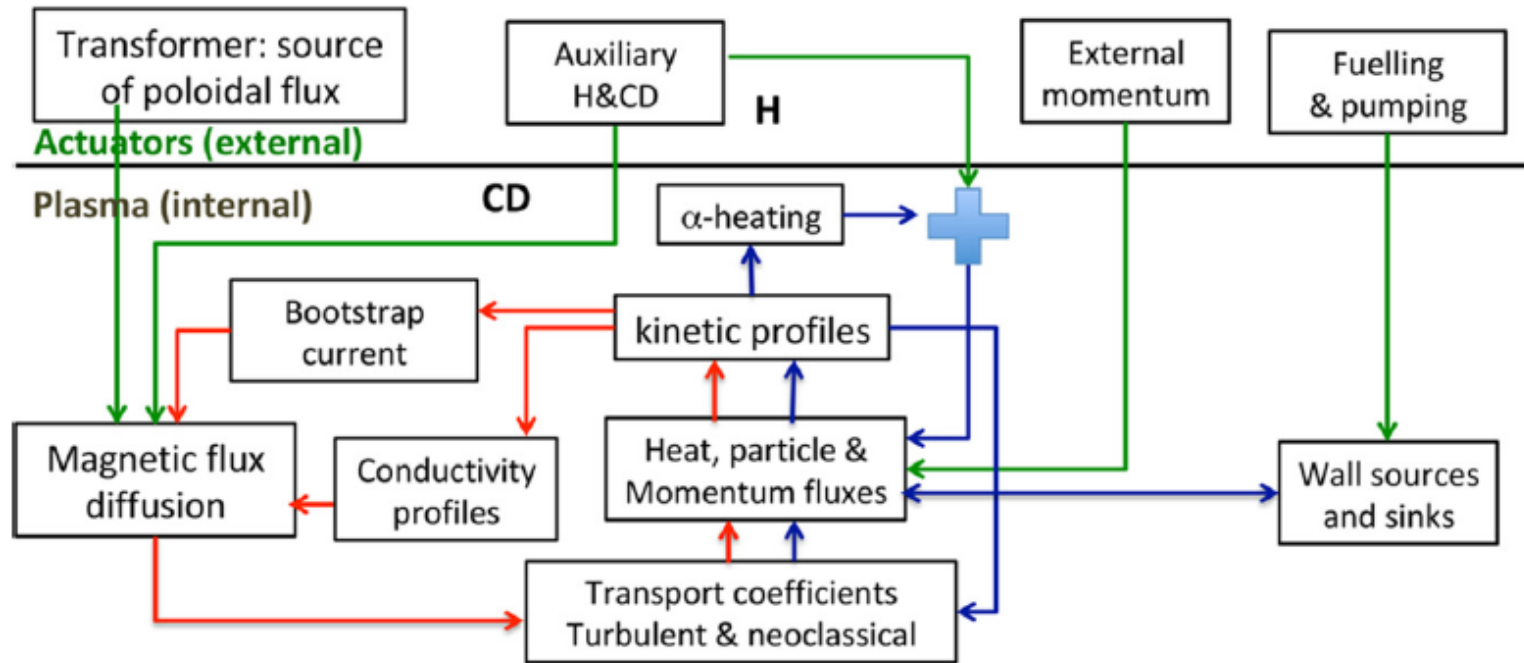
EDGE2D-Eirene [Reiter JNM 1992,
Simonini CPP 1994]

UEDGE [Rognlien JNM 1992] ... and others!

Overview of integrated tokamak modelling (multi-physics simulation)

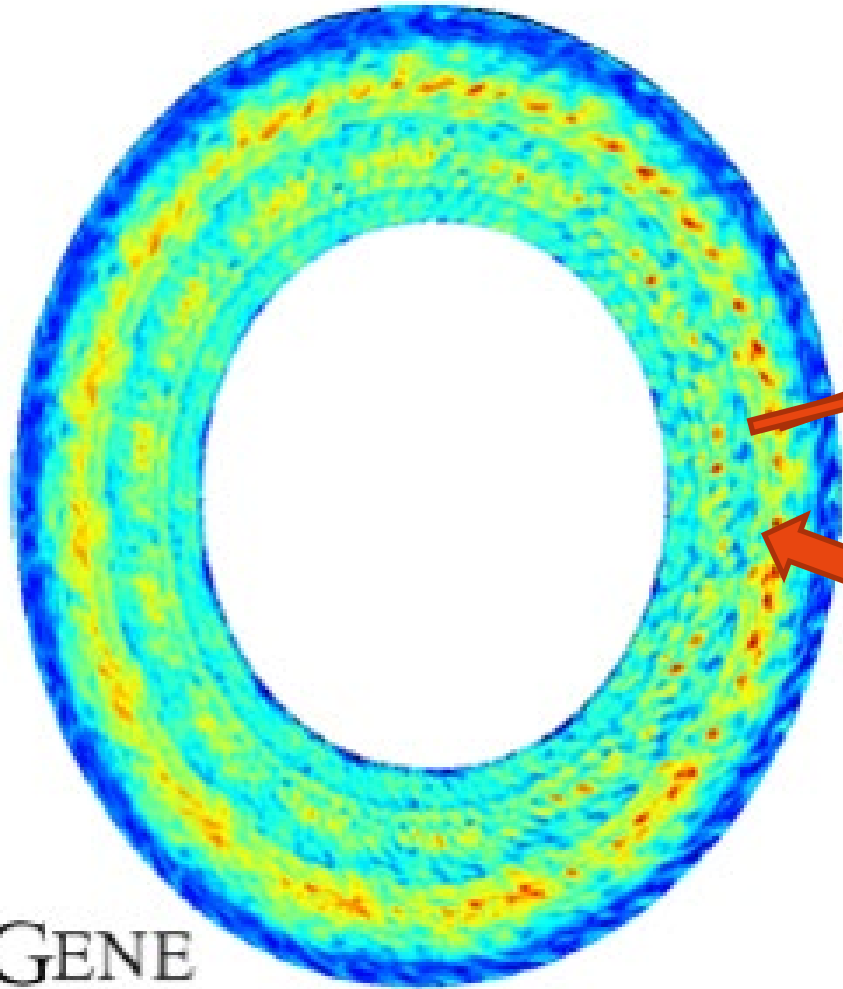


Multiple physics sub-components, multiple nonlinearities



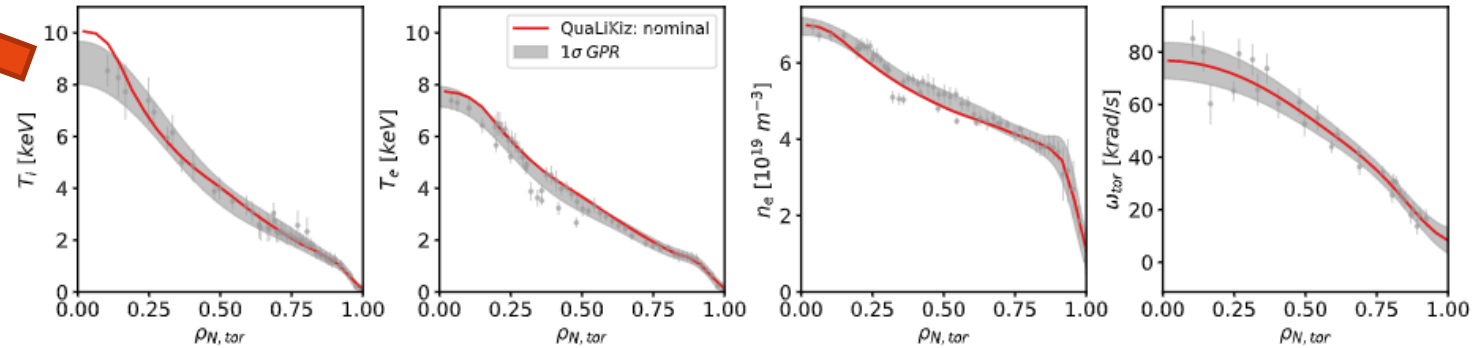
Kinetic profiles \equiv radial distributions of plasma temperature, density, angular momentum

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



Density,
temperature,
momentum

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



GENE

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



Subset of modelling use-cases

- **“Interpretative”**: get information from modelling unavailable from measurements, or to help constrain the measurements.
 - Heating and fuelling deposition profiles
 - Distribution of plasma electric current and magnetic fields
- **“Validation”**: predict profiles of temperature, density, impurities, rotation.
Do our physics models agree with the measurements?
 - UQ very important, of model settings and uncertainties of prescribed measured quantities in simulation (e.g. boundary conditions)
 - Allows physics understanding of mechanisms that lead to specific conditions
- **“Predict First”**: extrapolation to future performance (e.g. JET DT, ITER, DEMO)
- **“Optimization”**: experimental design, device design
- **“Controller design”**: Digital Twin of tokamak to design controllers
 - These use-cases demand *very* fast models, often ad-hoc.
Neural network surrogate models new direction in fast + accurate modelling

Components of the integrated tokamak simulator: Magnetic equilibrium



$$\mathbf{j} \times \mathbf{B} = \nabla p$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j}$$

$$\nabla \cdot \mathbf{B} = 0$$

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

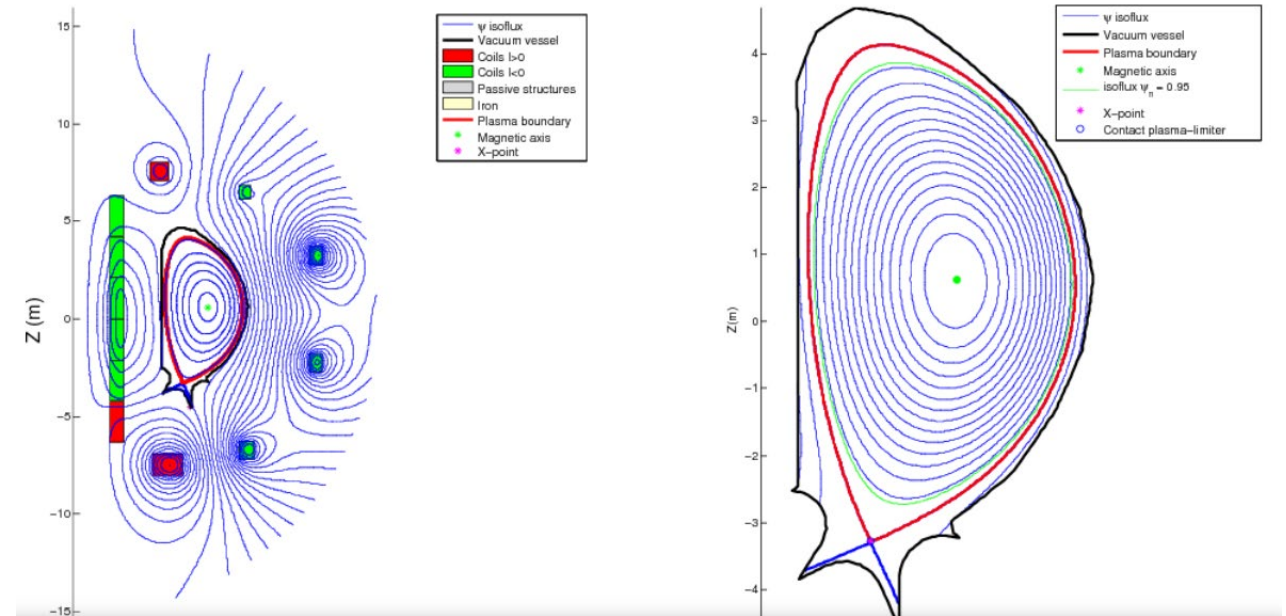
- Active coil circuits
- Induced plasma current
- Induced current in vacuum vessel

Coupled with electromagnetic equations for:

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

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

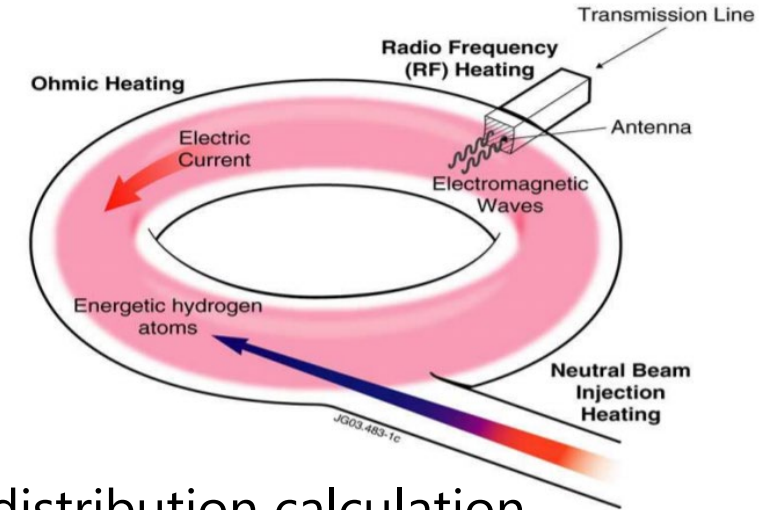


Heumann, Journal of Plasma Physics 2014

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)



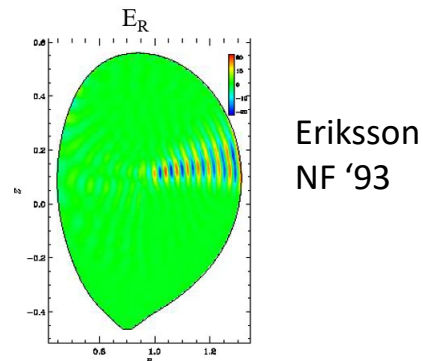
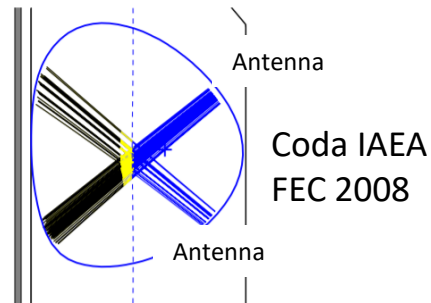
EM-wave calculations

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

Plasma Dielectric tensor $\overleftrightarrow{\epsilon}$ from kinetic theory
 $\vec{j}_{ext} \equiv$ antenna current

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

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 \rightarrow 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

Perpendicular drifts due to e.g. field inhomogeneity (ordered lower than v_{\parallel})

Collision operator

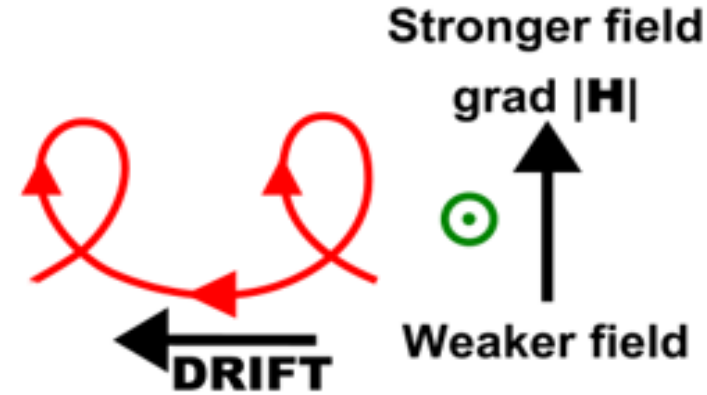
Static solution and perturbation around f_0 Maxwellian

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

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

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 perpendicular 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]



Gyrokinetic model of plasma turbulence

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

$$n = \int f d^3v$$

$$\mathbf{u} = \int \mathbf{v} f d^3v$$

$$T \propto \int v^2 f d^3v$$

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

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

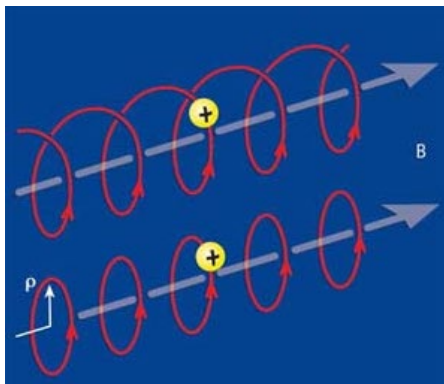
Leads to nonlinearity
(self-generated fields)

Field equations

$$\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{B} = \frac{4\pi}{c} \sum_j q_j \int \mathbf{v} f_j d\mathbf{v} + \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t}$$

$$\nabla \cdot \mathbf{E} = 4\pi \sum_j q_j \int f_j d\mathbf{v}$$



(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”



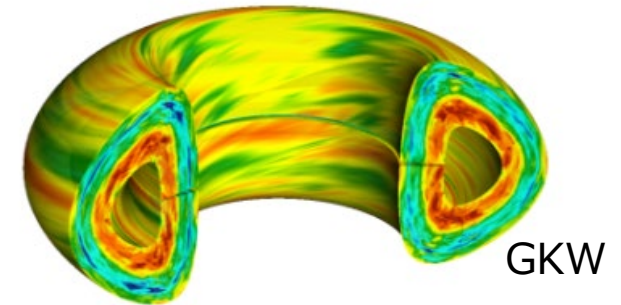
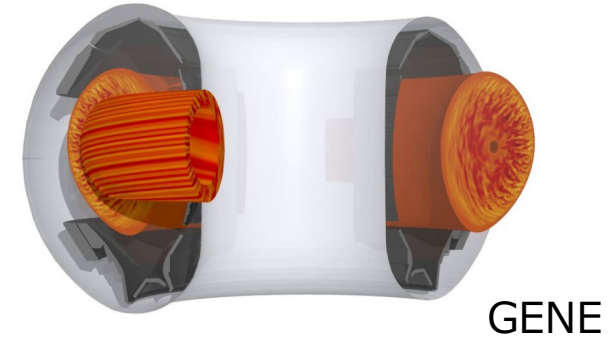
Multiple groups and codes worldwide working on simulations and interpretation of gyrokinetic turbulence and comparison with experiment

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

GENE (www.genecode.org)

GKW (<http://www.gkw.org.uk>)

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

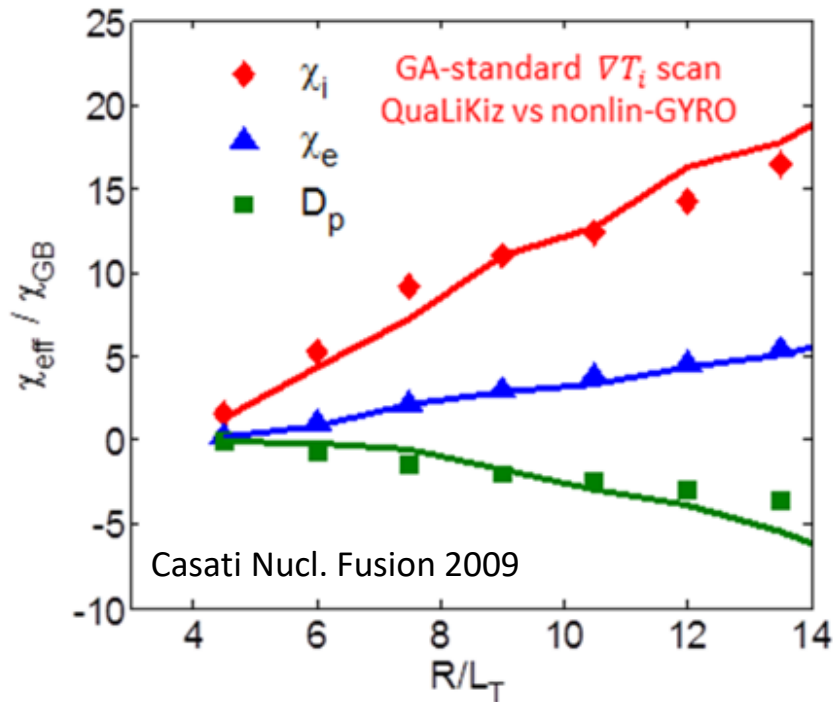


But... simulations too expensive and slow for routine use for modelling and optimization of tokamak scenarios. $10^4 - 10^6$ CPUh for each evaluation!

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



Quasilinear vs nonlinear heat convection and particle diffusion comparison



- 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]

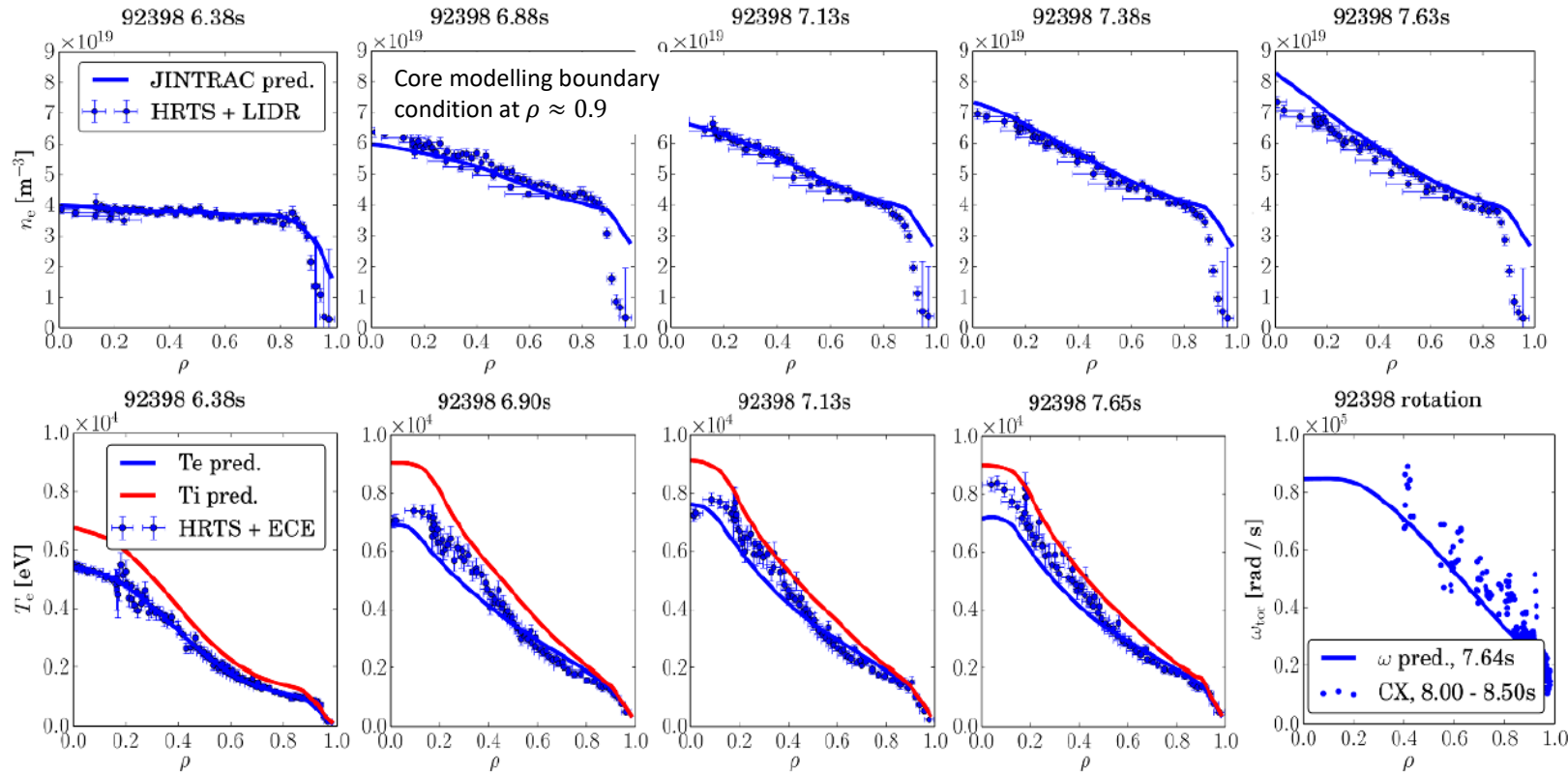
QuaLiKiz [Bourdelle PPCF 2016, Citrin PPCF 2017, Stephens JPP 2021, www.qualikiz.com]



Up next: case studies

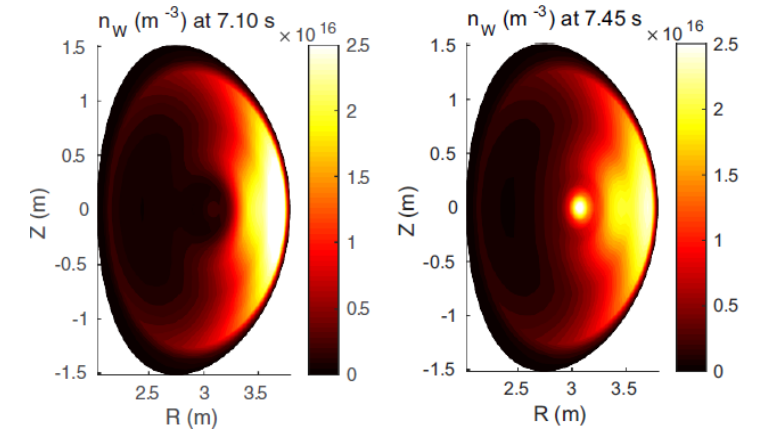
- Integrated modelling application at JET: modelling of impurity W plasma penetration
- Development of a fast and accurate turbulence transport modelling with neural networks

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



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



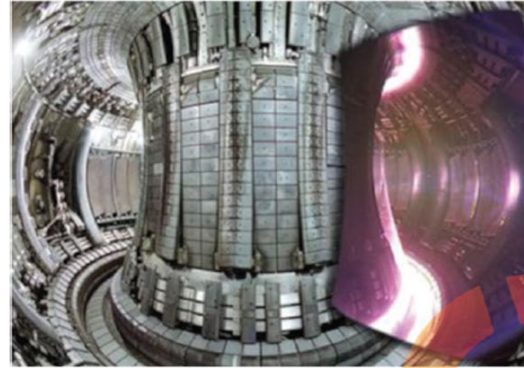
Neural networks learn the reduced turbulence model directly and replace it in tokamak simulation

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

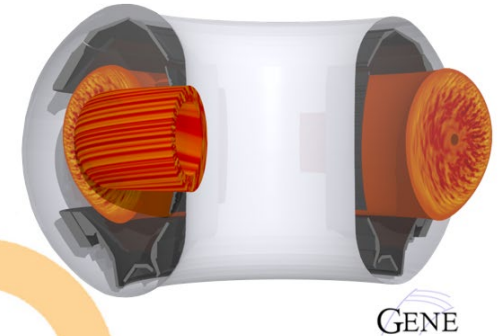
1. Quasilinear model tuned to nonlinear simulations and validated against experiments
2. Use to generate large datasets of turbulent calculations in relevant tokamak parameters
3. Feed-forward neural networks for regression of the model multivariate input-output map
4. Use the trained NN as a surrogate 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

1 second of plasma in...



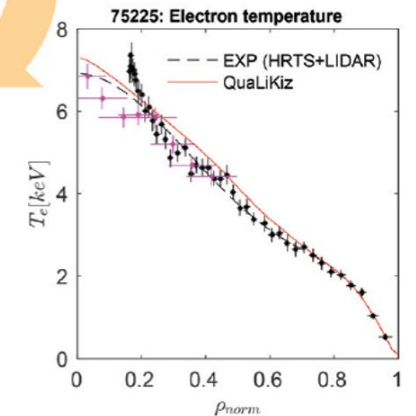
1 year on 1000 cores...



1 second on 1 core...



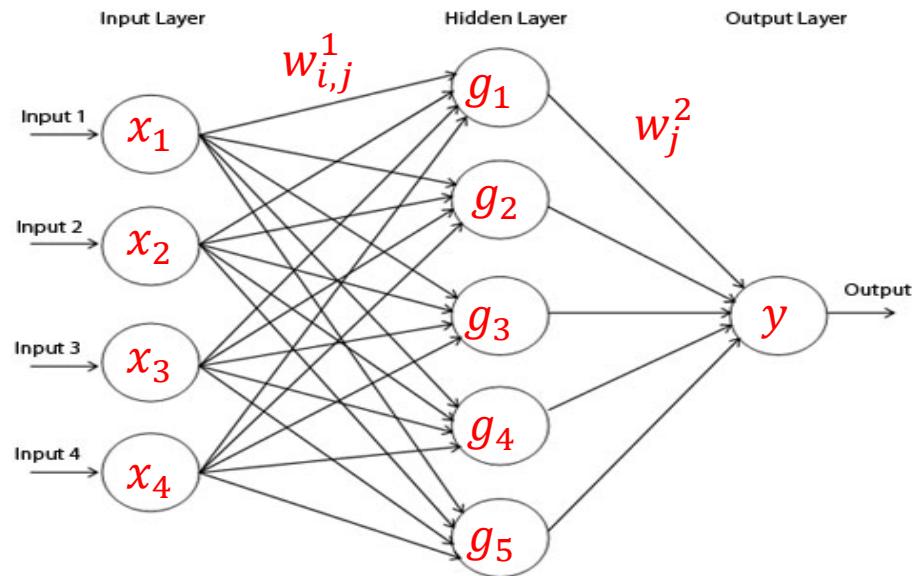
1 day on 24 cores...





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: $C = \sum_N (t_N - y_N)^2 + \lambda \sum (w_{ij})^2$

t_N are target values from generated dataset

λ is the regularization factor. Critical for avoiding overfitting

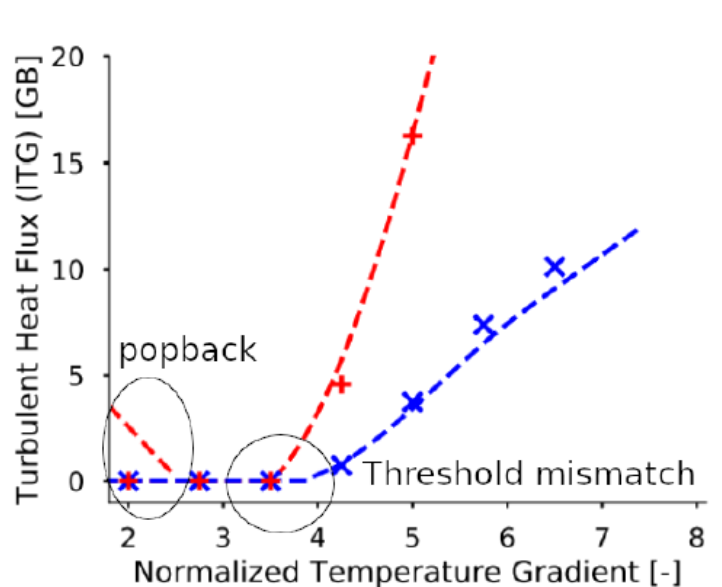
Additional advantage: provides an analytical formula with analytical derivatives. Turbulent flux derivatives with respect to inputs important for implicit timestep PDE solvers and trajectory optimization



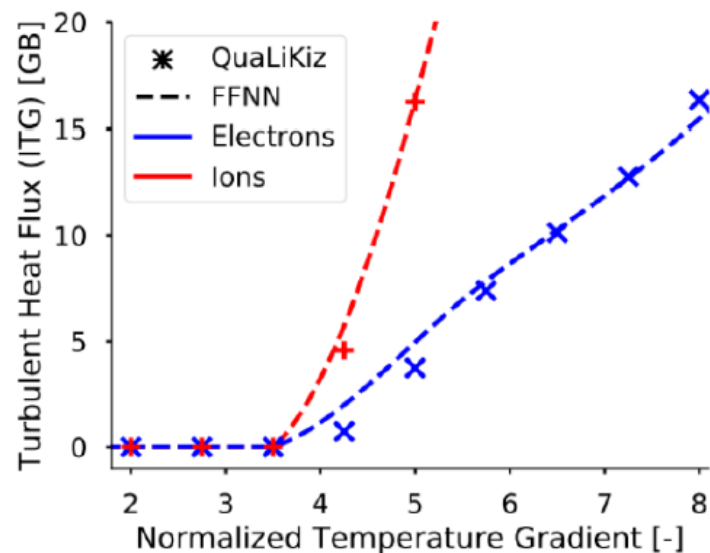
Key point is that RMS error is not a sufficient metric to determine quality of neural network fit. Emphy prior knowledge of system!

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

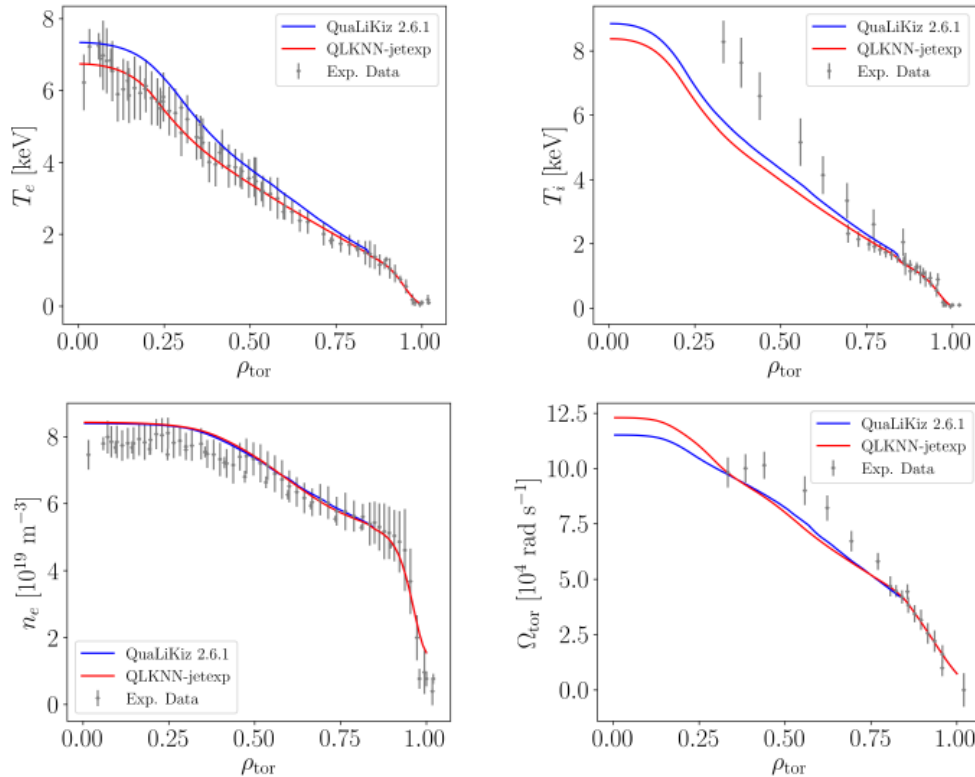


Good fit



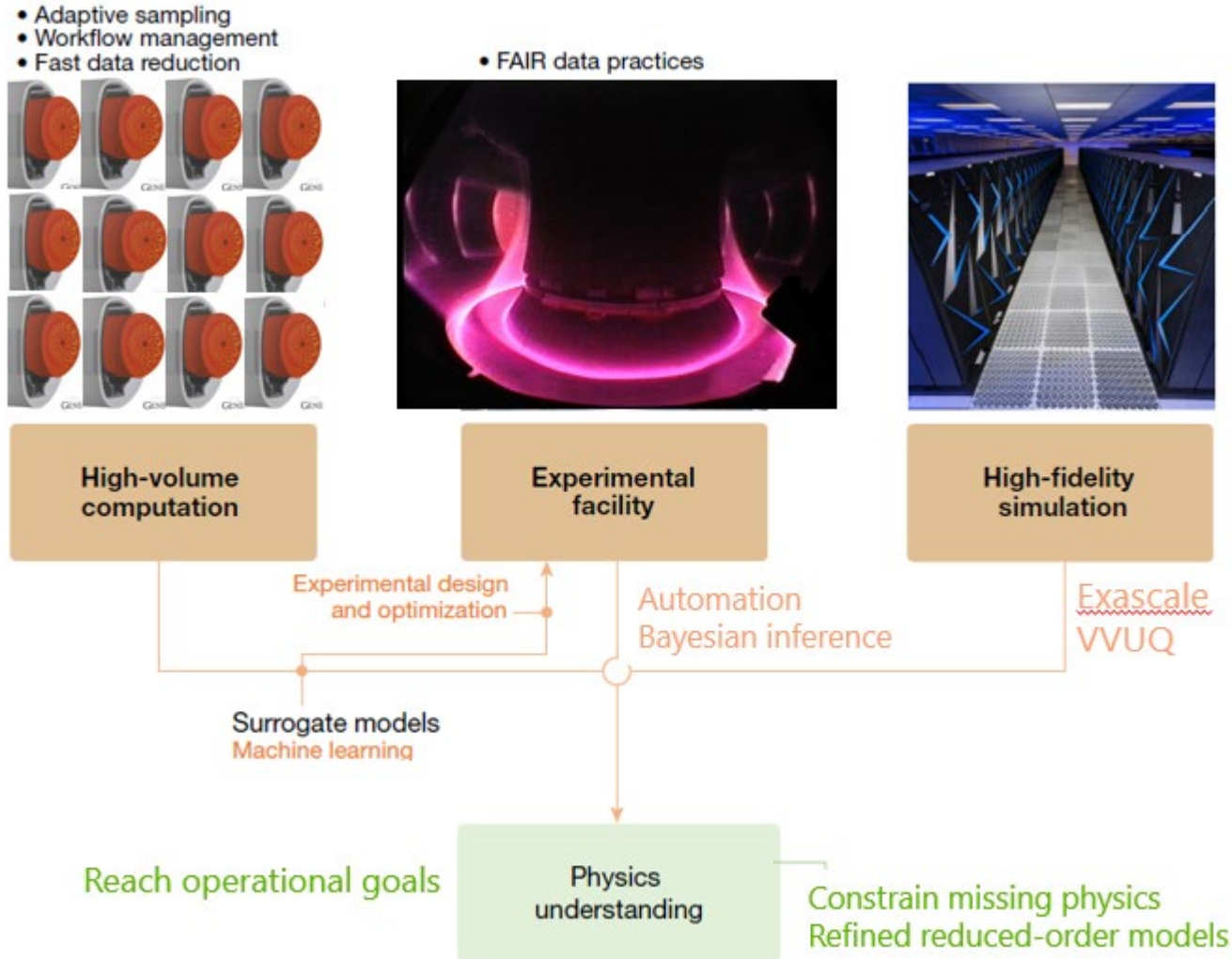
Case study: NN for turbulence surrogate model

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].
~ 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)

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





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