Particle-in-cell simulations of plasma-facing components for future thermonuclear reactors

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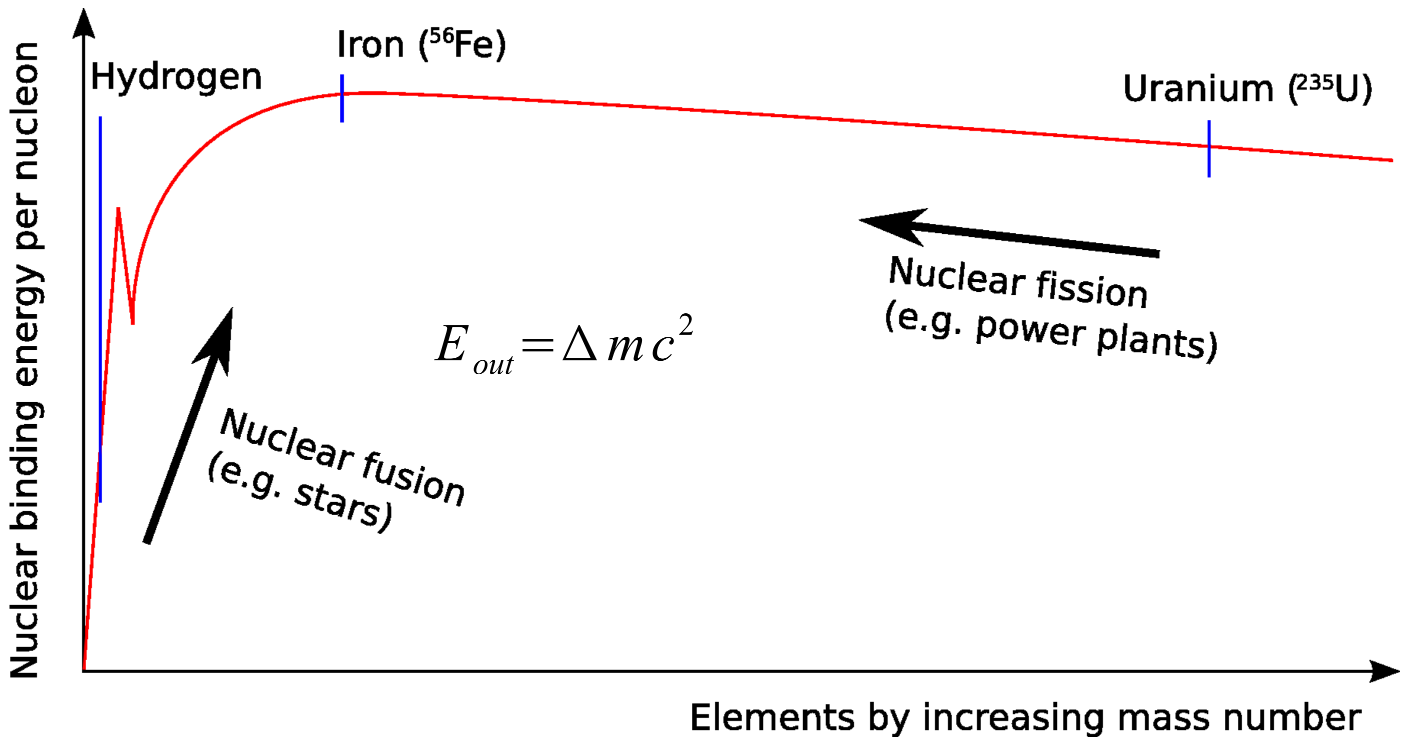
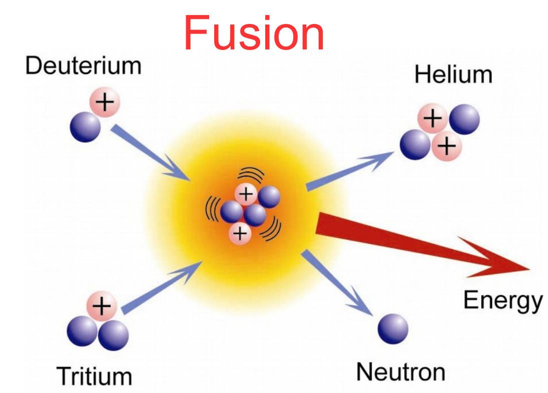
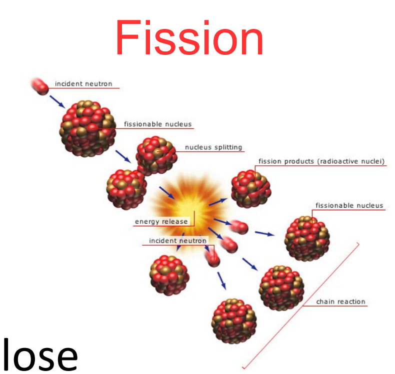
Outline

1. Introduction to nuclear fusion and magnetic confinement
2. Power exhaust problem
3. PIC simulations of poloidal gaps in ITER
4. Summary

Introduction to nuclear fusion







Nuclear fusion is a **nuclear reaction**, in which two (or more) atomic nuclei come close enough to form a new (heavier) product.

For elements with atomic number smaller than 56 (iron), this process is accompanied by a **release of energy**

Nuclear fusion is the source of energy in stars!

Can we achieve fusion on Earth?

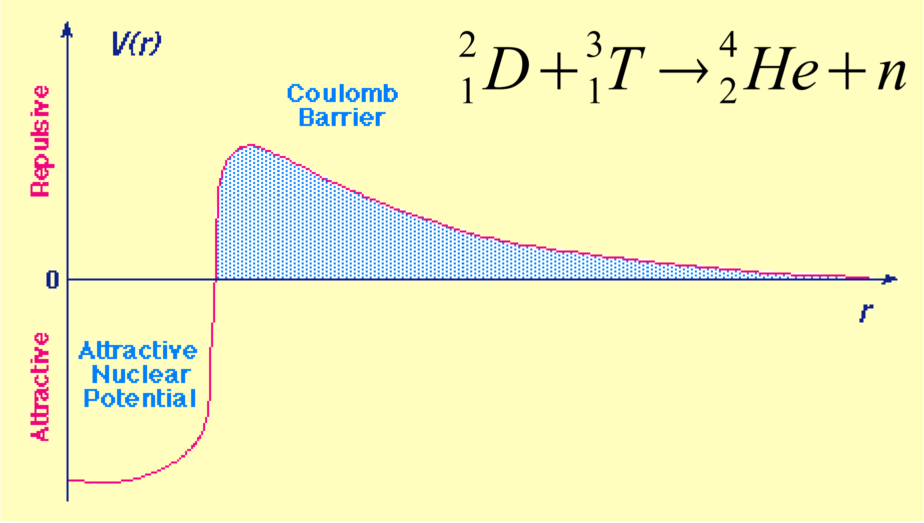
- Ions are **positively charged** – there is a **Coulomb barrier** preventing them from fusing

- Two principal methods of achieving fusion reaction:

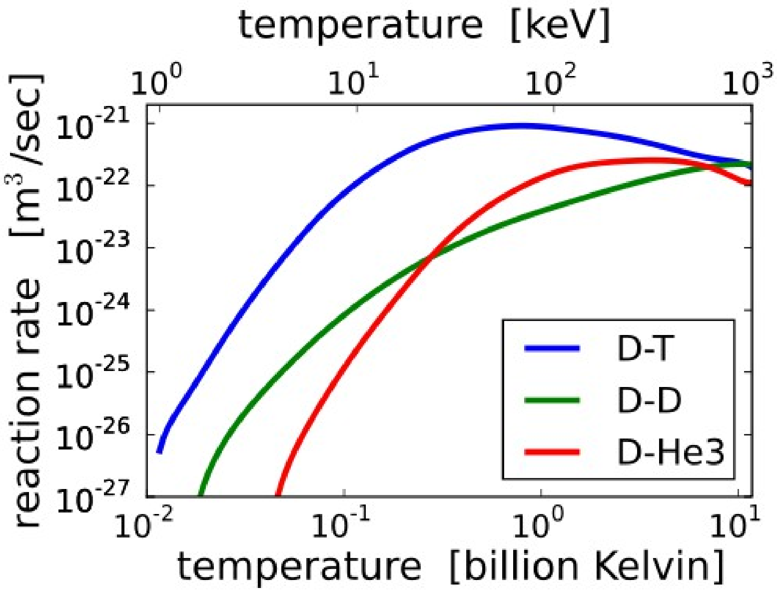
1. **Accelerated ions** bombard solid target or two ion beams collide – first demonstrated by Mark Oliphant in 1932. Problem: only few head-to-head collisions occur

2. Heat ions to **high temperature** so that their thermal collisions lead to fusion

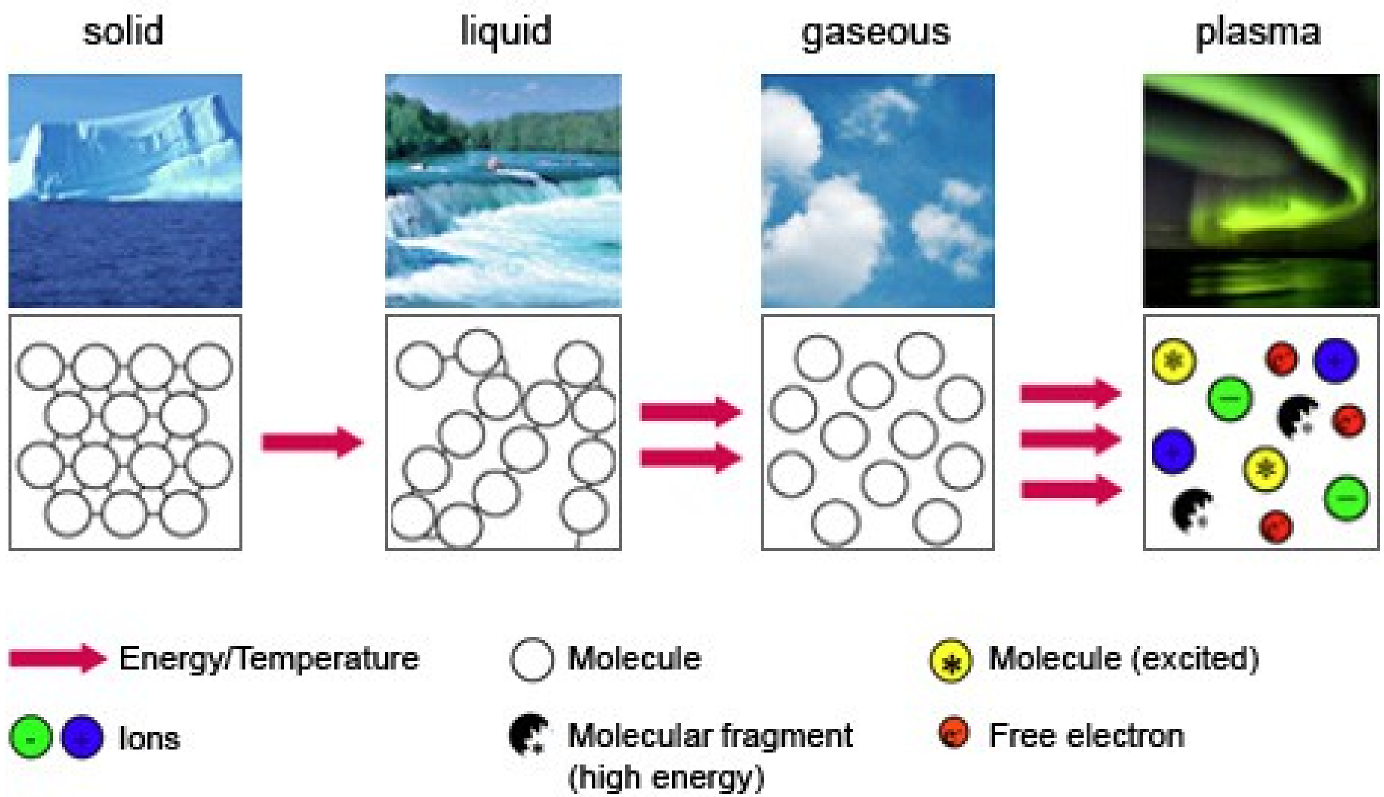
- Each reaction has different barrier magnitude, **DT fusion** is the easiest



$${}^{2}_{1}D + {}^{3}_{1}T \rightarrow {}^{4}_{2}He + n$$



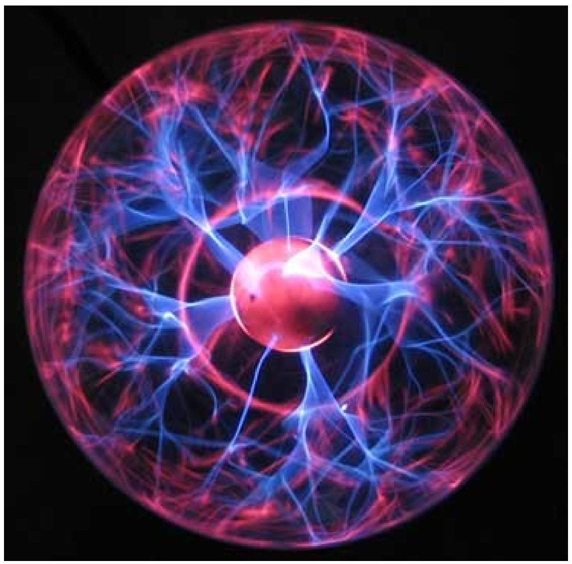
Matter at 100 000 000 Kelvin = Plasma



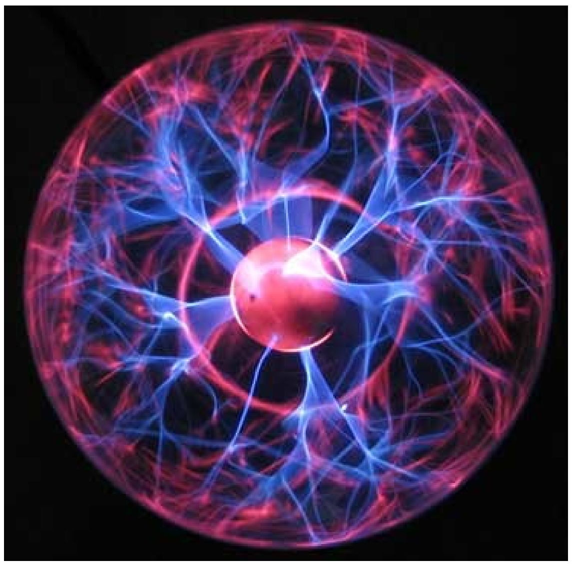
- Plasma contains significant fraction of **charged particles** – reacts to E and B fields

- Plasma may seem to be rare but in fact more than **99% of matter** in space is in plasma state!

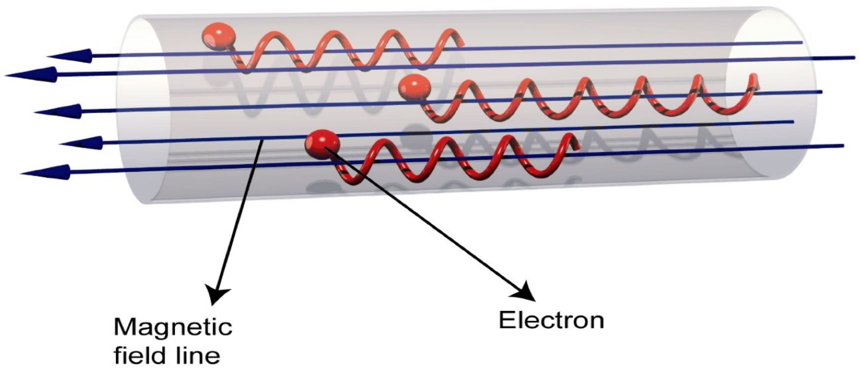
How does plasma look like?



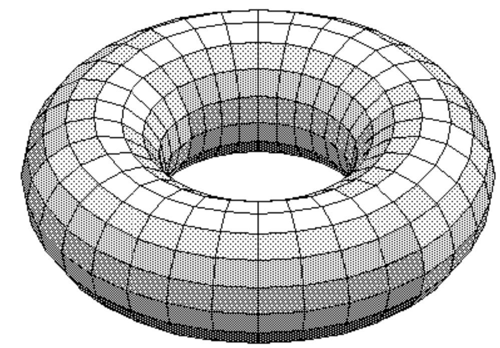
How does plasma look like?



Plasma confinement

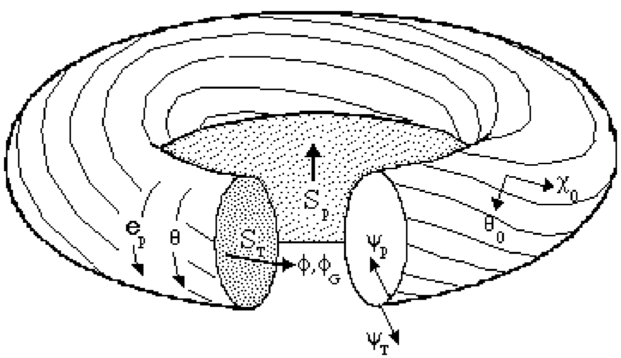


Torus



Objective: build a fusion reactor = stable source of energy with abundant fuel, which is economically viable

Twisted field lines



- Hot plasma must not be in contact with **reactor wall**
- Charged particles in magnetic field follow **helix trajectory**, which **restricts motion** across the magnetic field lines
- Field lines can be closed by formation of a **torus**
- In order to prevent instabilities, the field lines must be further **twisted**

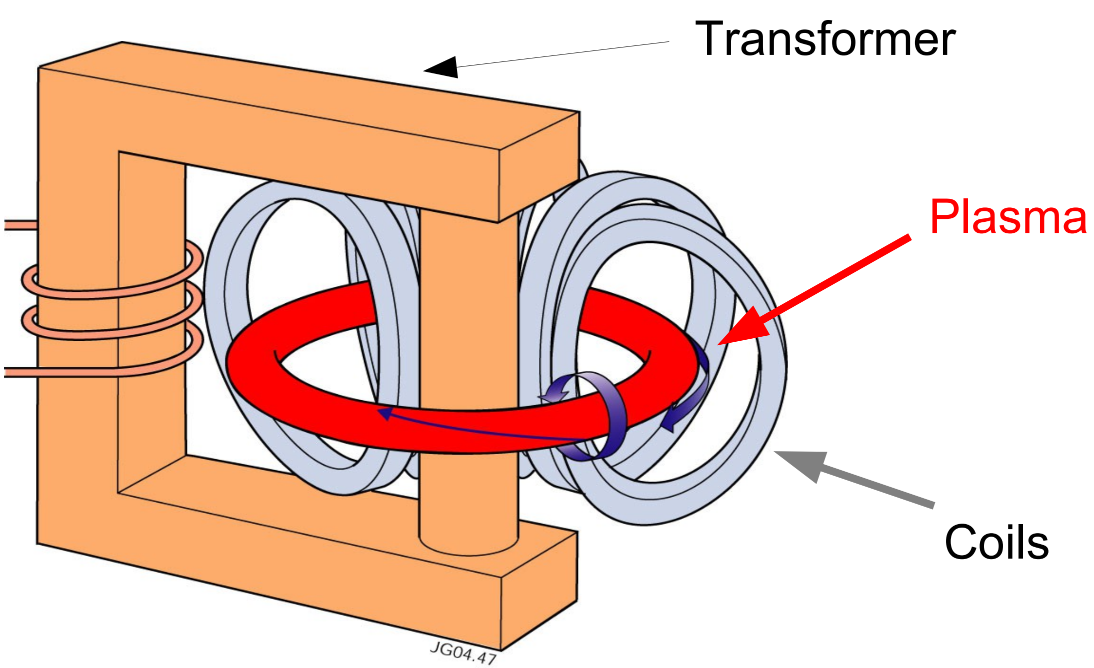
Tokamak – concept for magnetic confinement

- The magnetic field is created by combination of external coils **(toroidal field)** and electrical current passing through plasma **(poloidal field)**

- Originally, plasma current was driven by using plasma as a secondary winding of a **transformer**

- Nowadays, steady-state methods of **current drive** exists (discharges up to ~5 min)

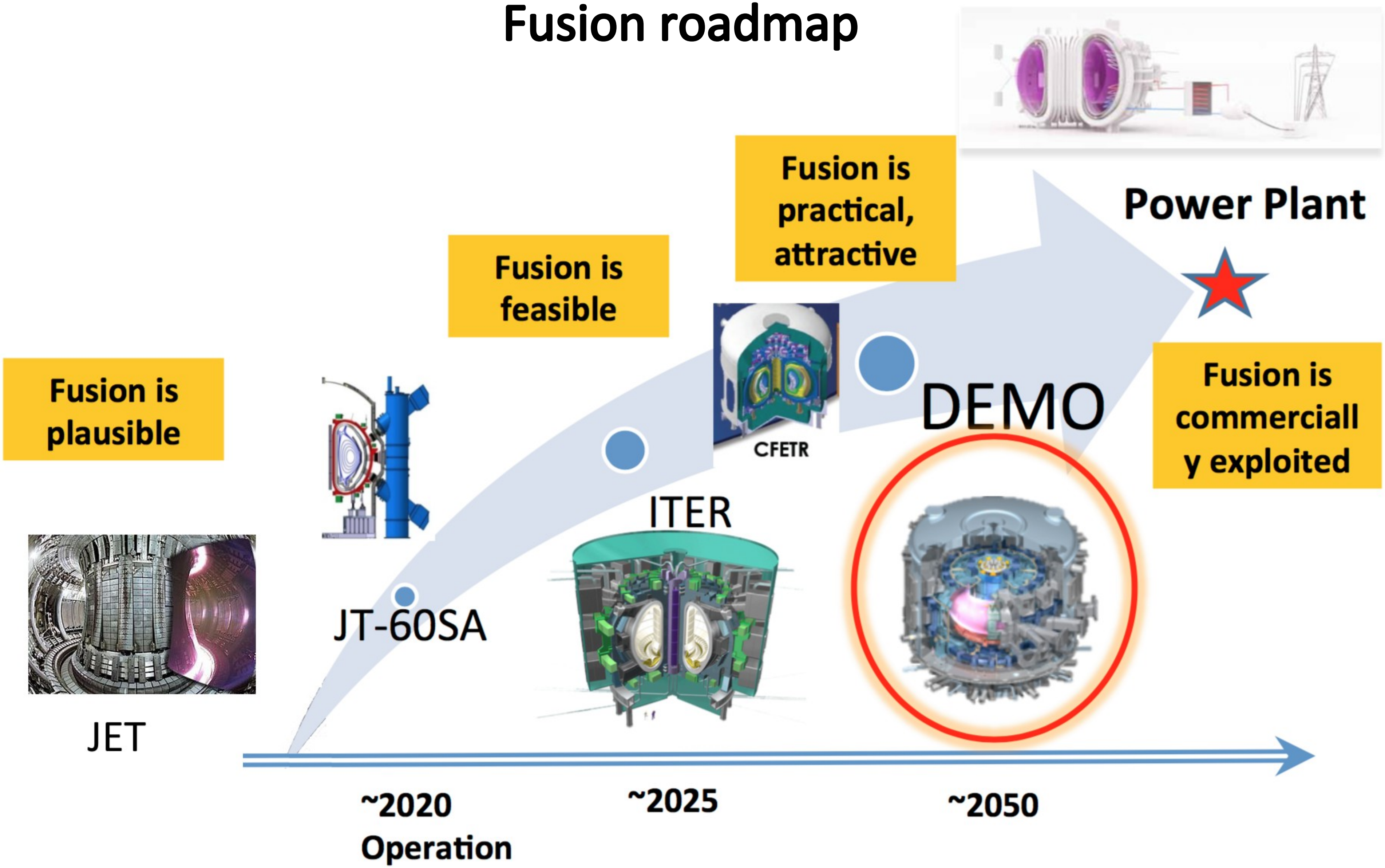
- Tokamak plasma can be heated by Ohmic power, RF waves or by injection of high energy neutral atoms (NBI)



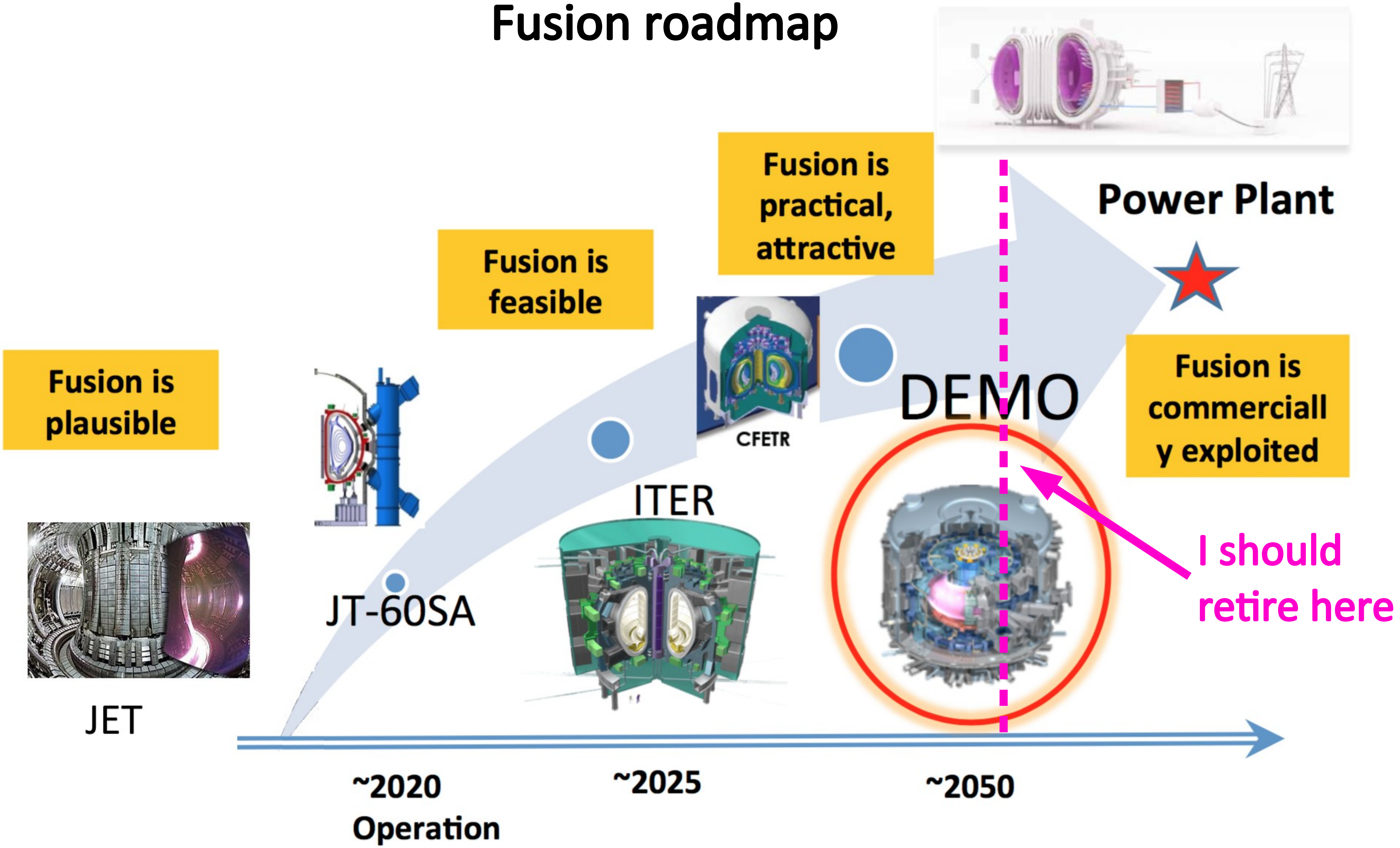
- Tokamak = *toroidal'naya kamera s magnitnymi katushkami*

- Soviet design from the '50s

Fusion roadmap



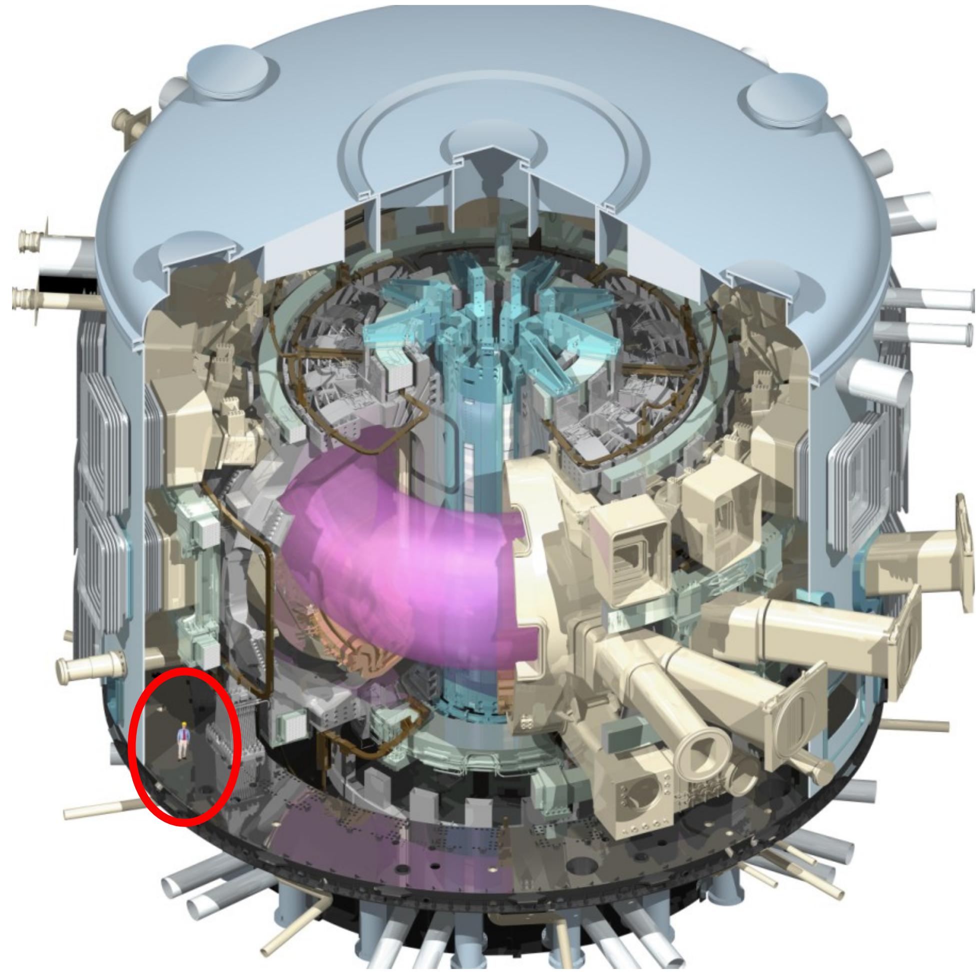
Fusion roadmap



Fusion research today – building ITER

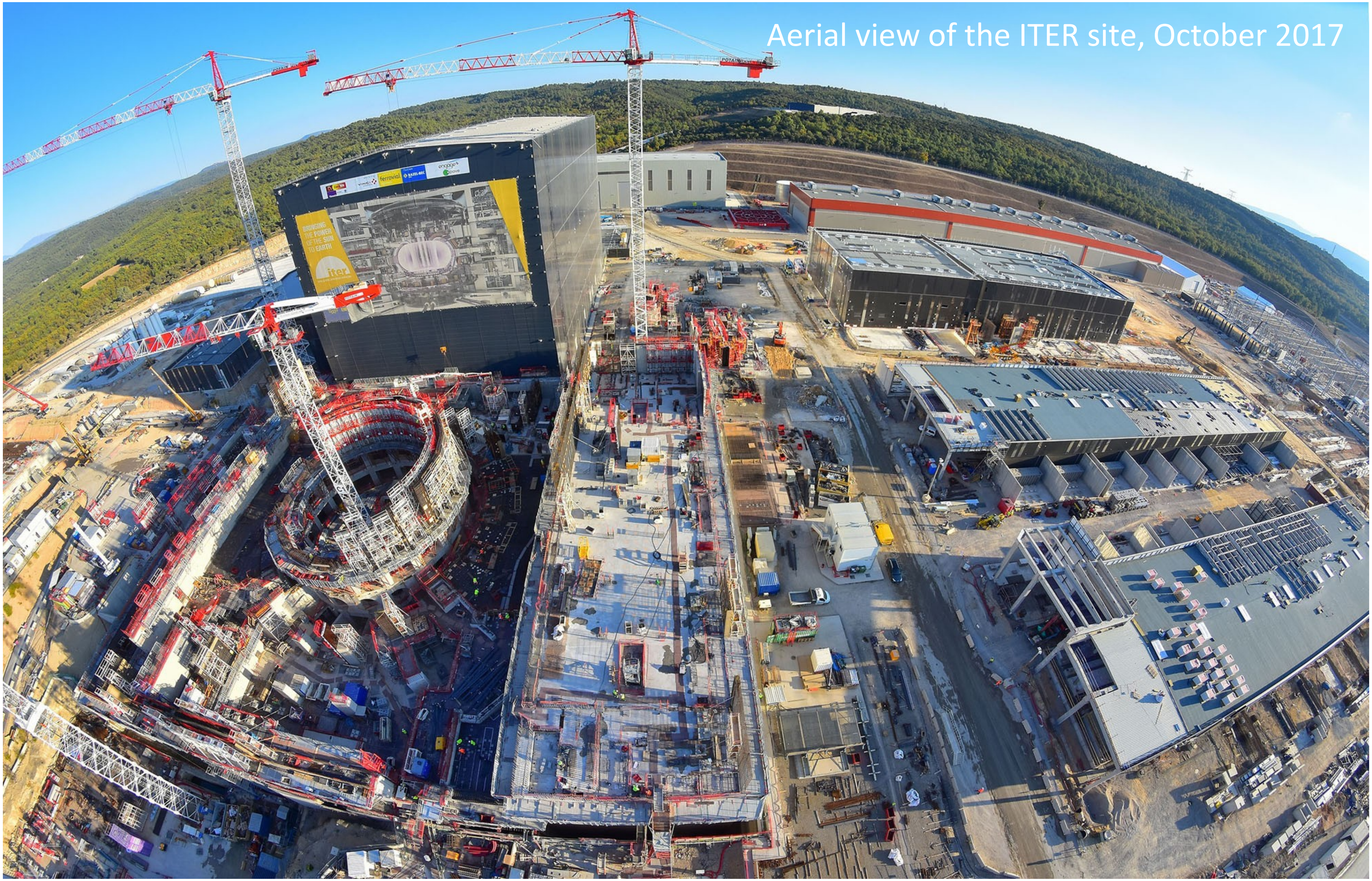
Parameters:

Cryostat height, diameter	~30 m
Major radius	6.2 m
Minor radius	2 m
Plasma volume	850 m^3
Plasma current	15 MA
Magnetic field	5.6 T
Pulse duration	~1000 s
Plasma heating	50 MW
Fusion power	500 MW
First plasma	2025
First DT plasma	2032

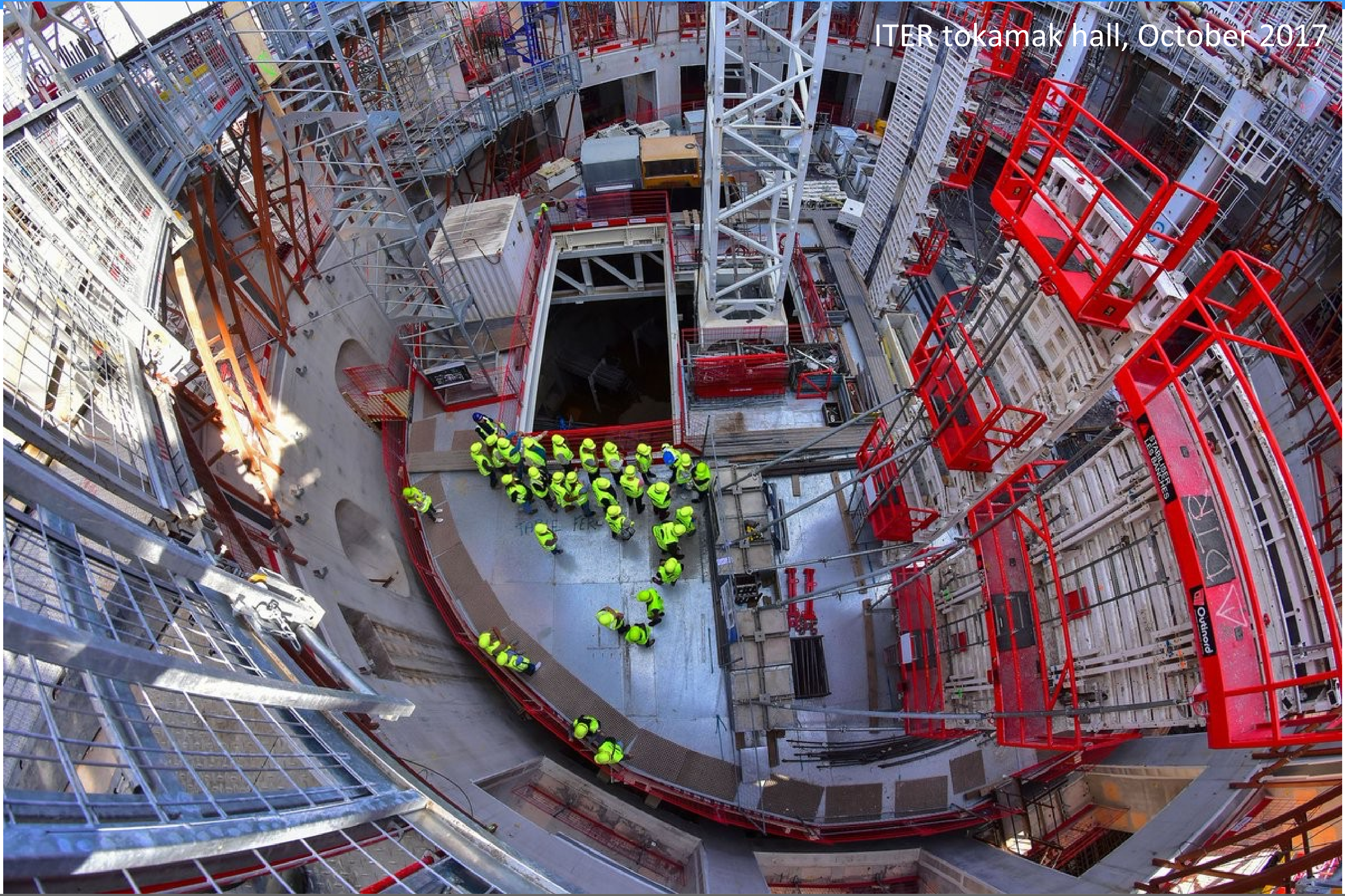


ITER should produce more energy than we put in!

Aerial view of the ITER site,September 2017



Aerial view of the ITER site, October 2017

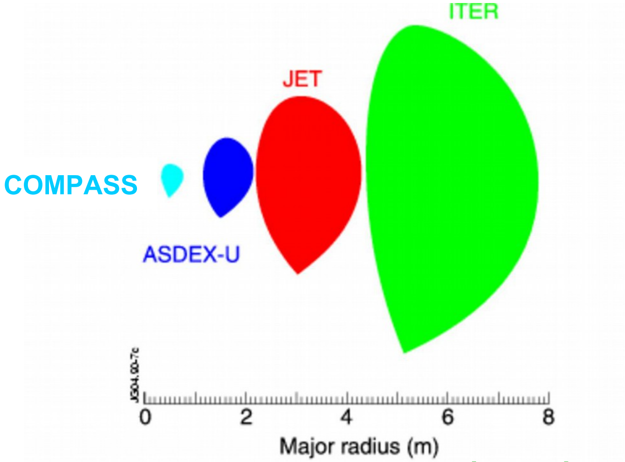


ITER tokamak hall, October 2017

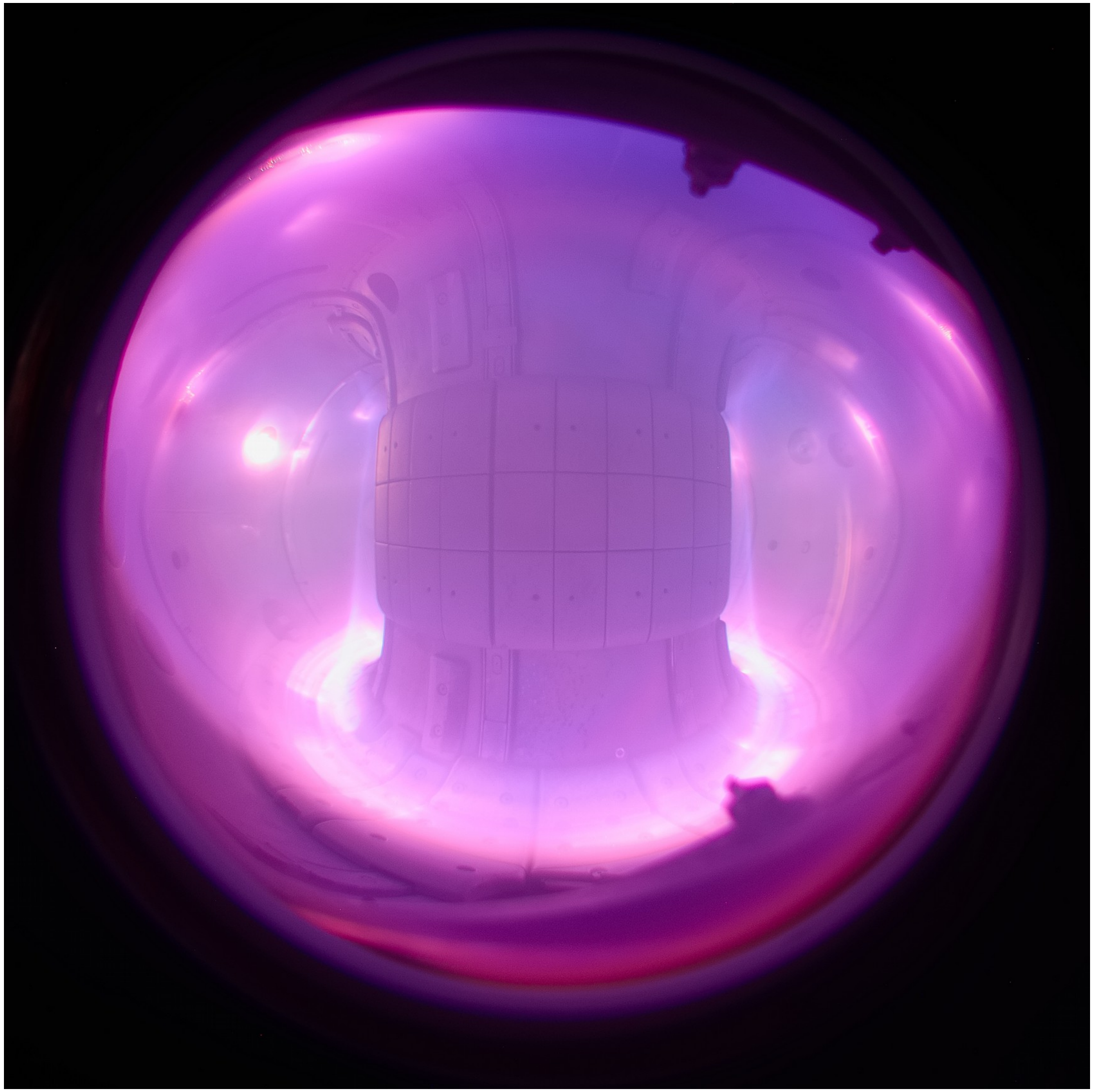
Fusion in Prague - tokamak COMPASS

Parameters:

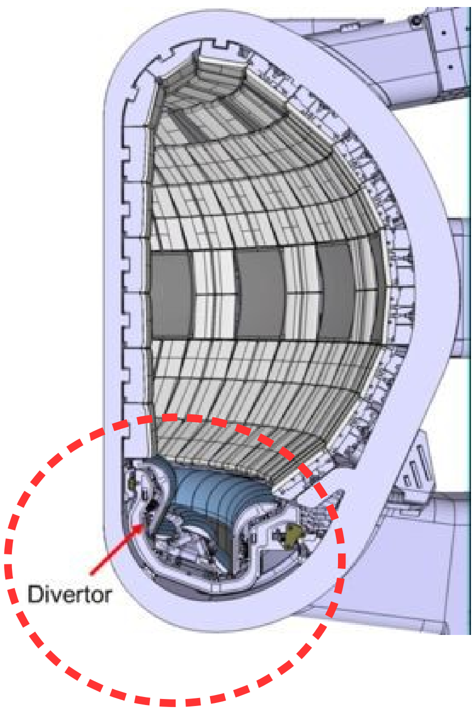
Major radius	0.56 m
Minor radius	0.2 m
Plasma volume	~1 m^3
Plasma current	up to 350 kA
Magnetic field	up tp 1.6 T
Pulse duration	< 0.5 s
Plasma heating	2*0.3 MW (+ 1 MW planned in 2019)



ITER-like geometry (1:10)



Power exhaust problem – ITER divertor



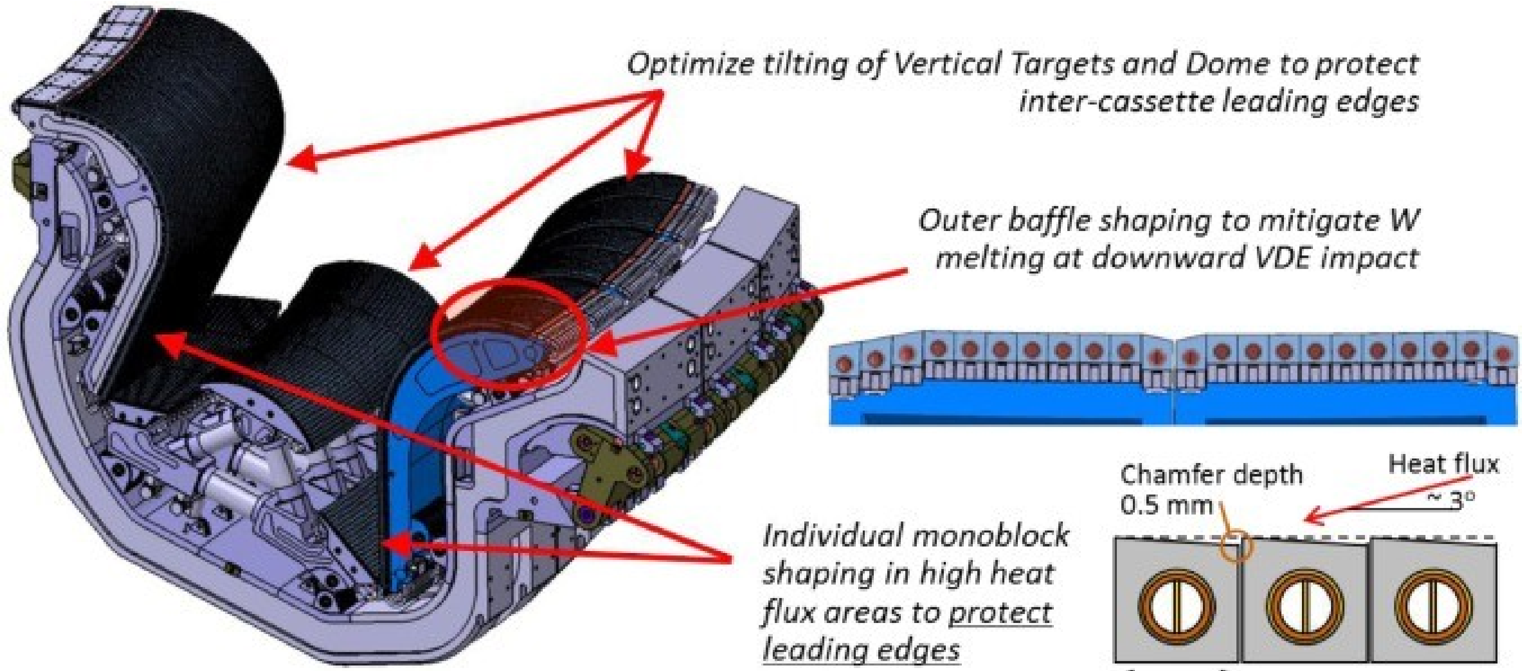


Figure: courtesy of T. Hirai et al. NME 2016

- Most of the heat flux is deposited at the bottom of the machine in the **divertor**
- ITER divertor will be castellated – split into **monoblocks**, which are attached to cooling pipes
- The water-cooled W monoblocks have to handle **10 MW/m^2** of steady-state impinging heat flux (surface of the Sun emmits 60 MW/m^2)
- monoblock surfaces are at grazing angle with respect to B field to spread power -> **leading edges**

ITER divertor monoblocks – poloidal gaps

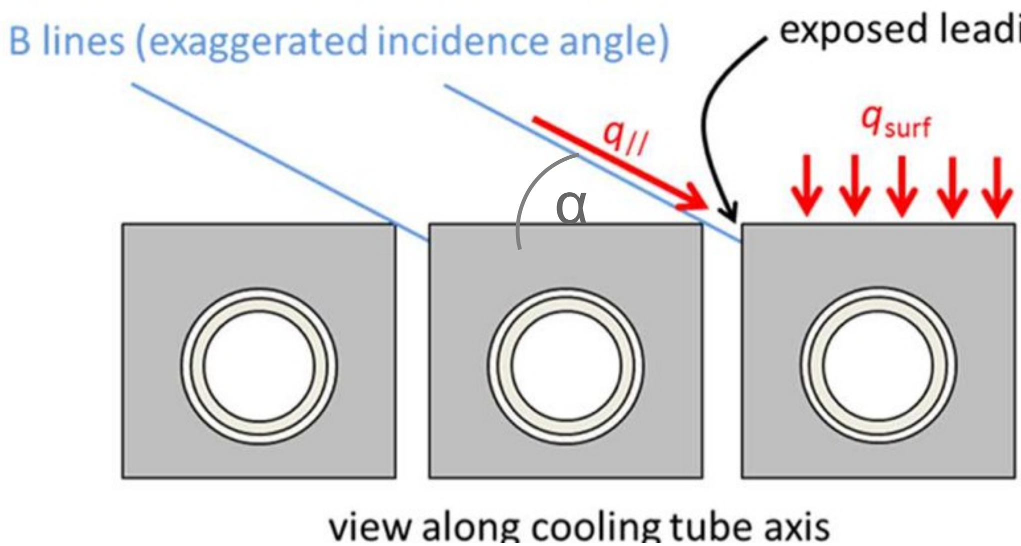
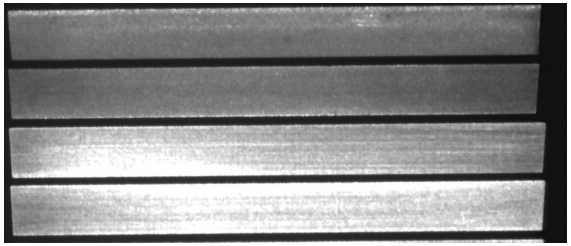
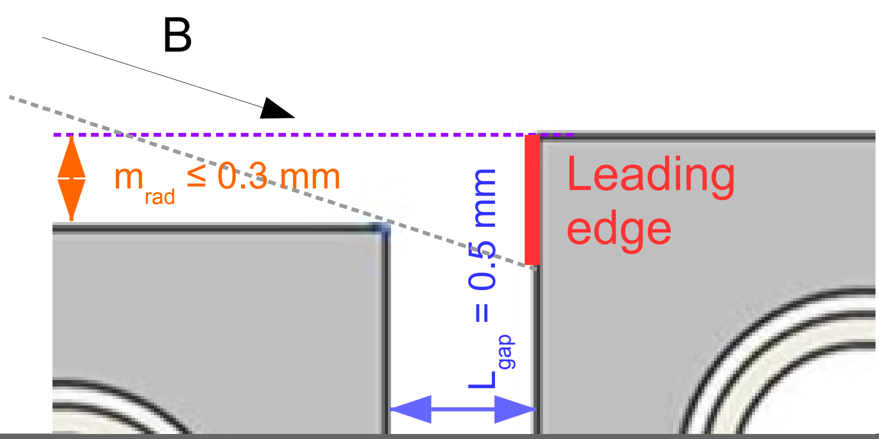


Figure courtesy of J.P. Gunn, IAEA 2014

- Incident angle ~2.7° (IVT), 3.2° (OVT)
- MB dimensions: 28 mm long, **0.5 mm gaps**
- Material: tungsten (highest melting point **3695 K**)
- BUT – looses favourable material properties if forced to recrystalize (~**1500 K**)

Tunsten lamella melting experiment at JET



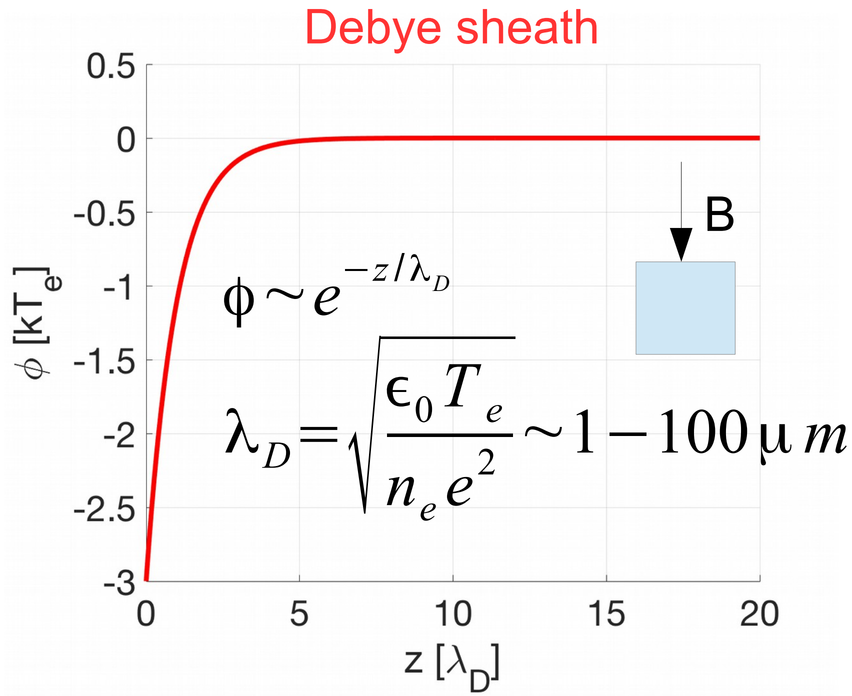


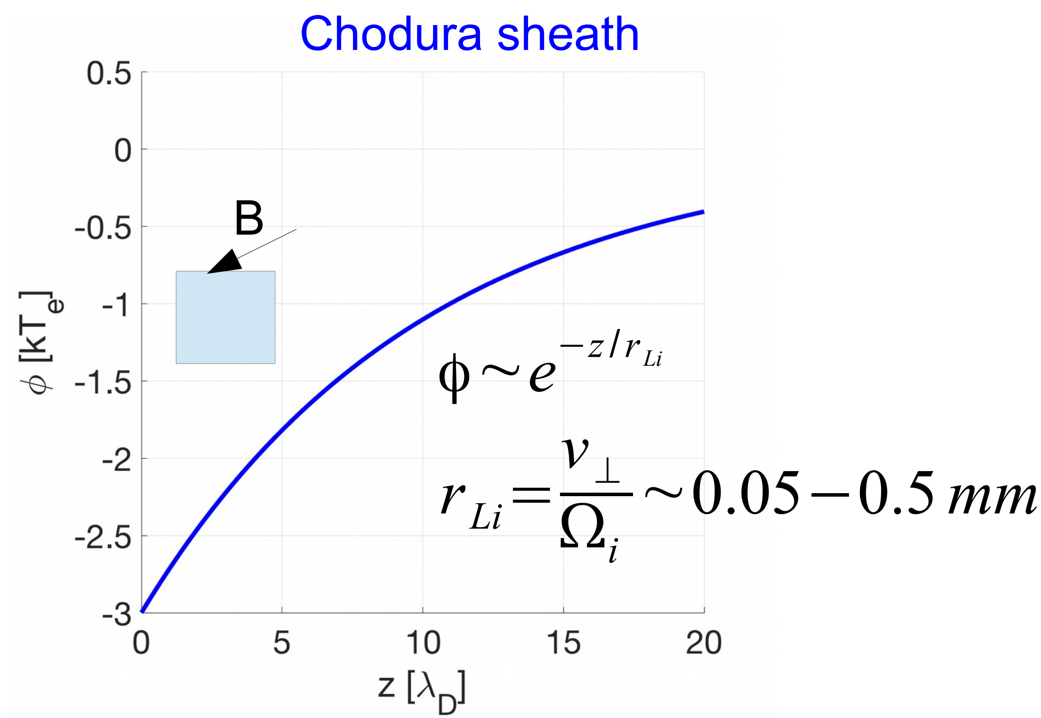
Engineering tolerances ensure that the **radial misalignment** between two neighboring monoblocks $m_{rad} \leq$ **0.3 mm**. This however significantly increases the area of the exposed leading edge

Will the monoblock melt at this location?

Plasma in contact with solid objects

- Electrons have much higher mobility due to smaller mass –> larger currents
- Floating conductor requires equal ion and electron current from plasma: electric field close to surface which repels most of the electrons = **Debye sheath** ~λ_D (Debye length)
- For B field at grazing incidence: **Chodura sheath** formation ~r_{Li} (ion Larmor radius)





- In tokamak plasmas r_{Li}/λ_D = 5 - 50

How to study the monoblock power loading?

Different approaches with very different computational complexity

1. Optical model

Assumes that power flux is deposited only on the magnetically exposed areas and that the magnitude is given by the surface orientation with respect to the B field $q_{surf} = q_{\parallel} \sin(\alpha)$

2. Ion orbit model

Monte-carlo simulation: follows ion trajectories in a given geometry. Plasma conditions determine the initial velocity distribution function. E field is not considered, B field static. Trajectories have analytical form (helices), number of particles only determined by required precision of the profiles.

3. Particle-in-cell model

Follows ions and electrons in self-consistent E field and static B field. Includes both finite Larmor effects and sheath E field but very computationally demanding – needs to follow up to ~200 milion particles during ~10 million time steps.

Particle-in-cell technique

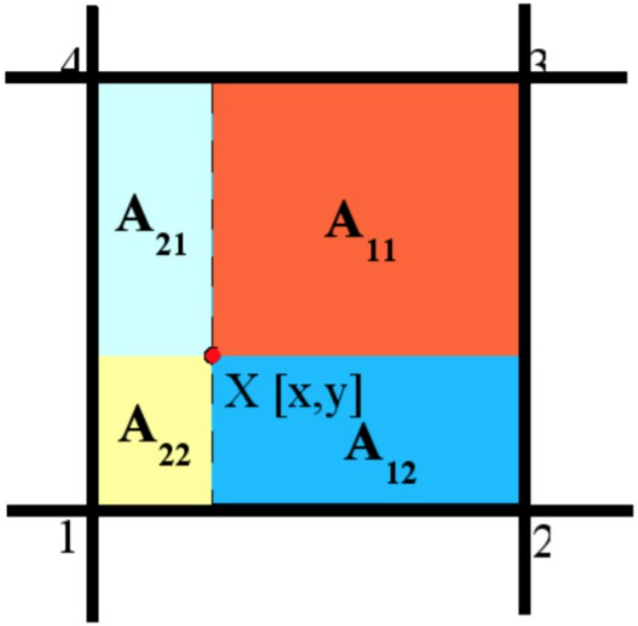
- Solves the equation of motion of individual particles (or macroparticles) in each time step

$$\frac{dv}{dt} = \frac{q}{m}\left(E + v \times B\right)$$

- **B field** is imposed, **E field** calculated from Poisson's equation – given by **charge density** created by the particles (ions and electrons)

$$E = -\Delta \frac{\rho}{\epsilon}$$

- The charge density of particles is approximated by a grid –> collective field acting on all particles -> complexity ~N log(N) instead of ~N^2 for true N-body system



-Limits of the method determine the computational complexity:
1. The size of the cell in PIC grid should be ≤ λ_D
2. There should be at least 50 particles in each cell
3. Particle should not cross more than 1 cell during 1 time step

Sheath Particle-In-CEll codes

Collaboration between IPP Prague and CEA Cadarache

- Written in **fortran 90**, output in Matlab MAT files
- Standard PIC features: **leapfrog** for particle advancing, **cloud-in-cell** for weighting
- Parallel ion velocity distribution function – output of 1D kinetic code modelling pre-sheath
- Injection box: allows to handle B field at **grazing incidence**
- Parallelization: all components except for the Poisson solver, scaling up to **64 cores**
- Typically **100 000 – 10 000 000 time steps** required (< 1 μs of simulated time)
- Relatively long runtimes limited by parallelization: **10-100 days**
- Large memory requirements due to large number of particles ~**100 GB of RAM**

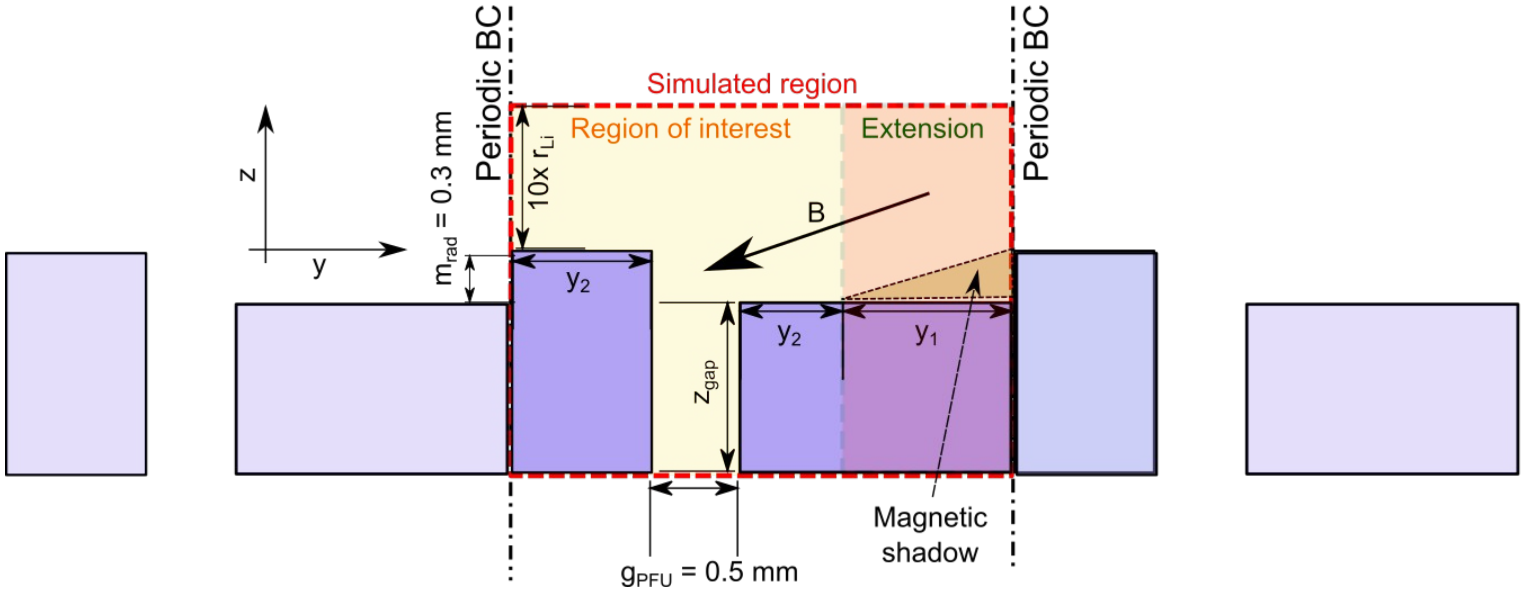
SPICE2

2D3V Cartesian code, direct Poisson solver (LU decomposition), grids < **4000x3000** cells

SPICE3

Full 3D3V code, multigrid Poisson solver, grids ~ **256x256x256** cells

2D simulations of poloidal gaps in ITER divertor



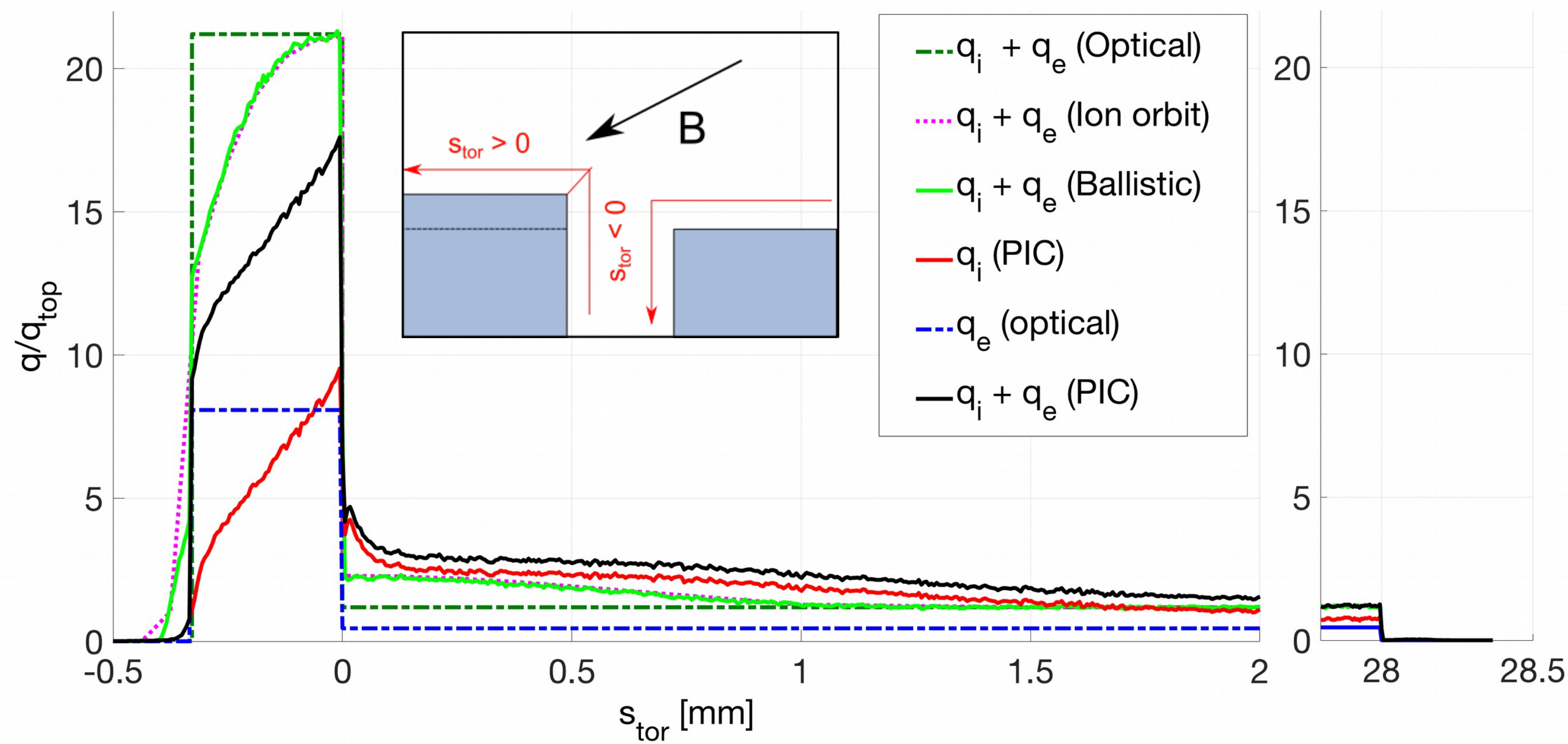
- Study requested by ITER Organisation and effectuated by IPP Prague
- Simulations performed at **IT4I** and **IFERC** (Japan)
- Geometry of the simulation: gap between monoblocks with radial misalignement
- Desired ouput: heat flux distribution along the monoblock surface
- Key questions:

How do sheath electric fields affect the result?

Can this problem be simulated by ion orbit model (which is much faster?)

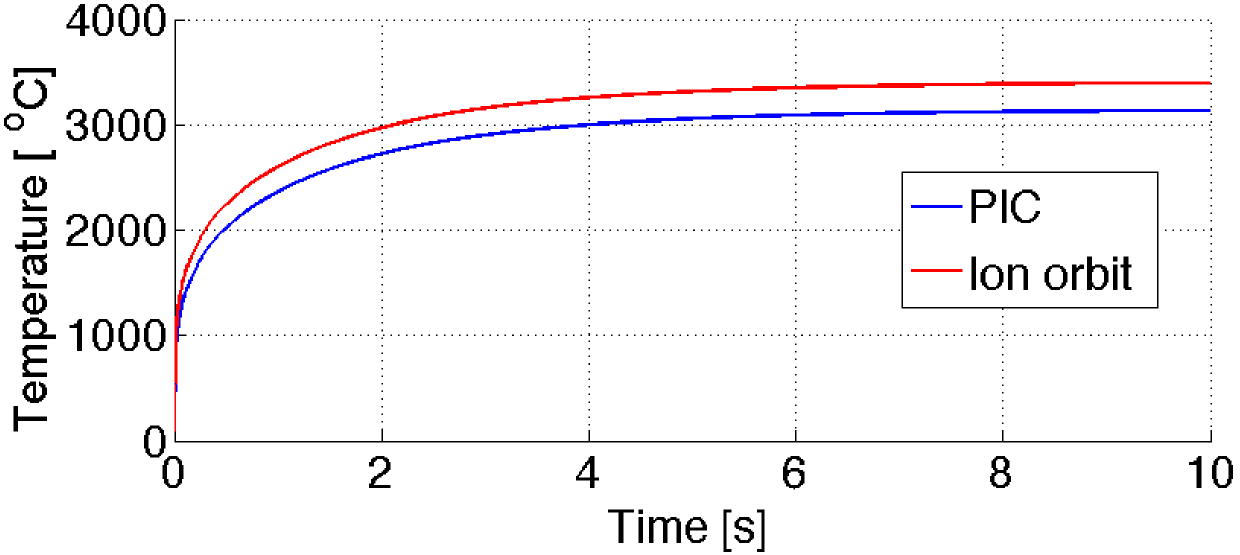
2D simulations of poloidal gaps in ITER divertor

- Comparison between the optical, ion orbit, ballistic (SPICE2 with E=0) and PIC model
- **Finite Larmor effect**: less power going to the leading edge, hits top surface instead
- This effect is increased when E field is taken into account – acceleration of ions in the sheath



Is the difference between PIC and ion orbit siginificant?

- What matters in practise is **monoblock temperature**
- Output of both codes used in finite-element simulation of monoblock heating
- Difference in peak temperature **~10%**, this is smaller than uncertainty in input parameters
- Conclusion: **ion orbit is a good tool for further studies** (monoblock shaping etc.)



More details in: J. P. Gunn et al. **57** *Nucl. Fusion* (2017) 046025
M. Komm et al. **57** *Nucl. Fusion* (2017) 126047

Summary & Outlook

- PIC simulations are suitable to predict plasma interaction with plasma-facing components although they are in general very computationally demanding

- We have effectuated a study for ITER organisation and verified that for the specific plasma conditions and geometry the **ion orbit code can be used** for optimisation studies

- A subsequent study led to a **change of design** of the ITER divertor monoblocks

- Current "hot" topics in the field:

1. Simulations of **thermionic emission** from hot tungsten surfaces (in 2D and 3D)

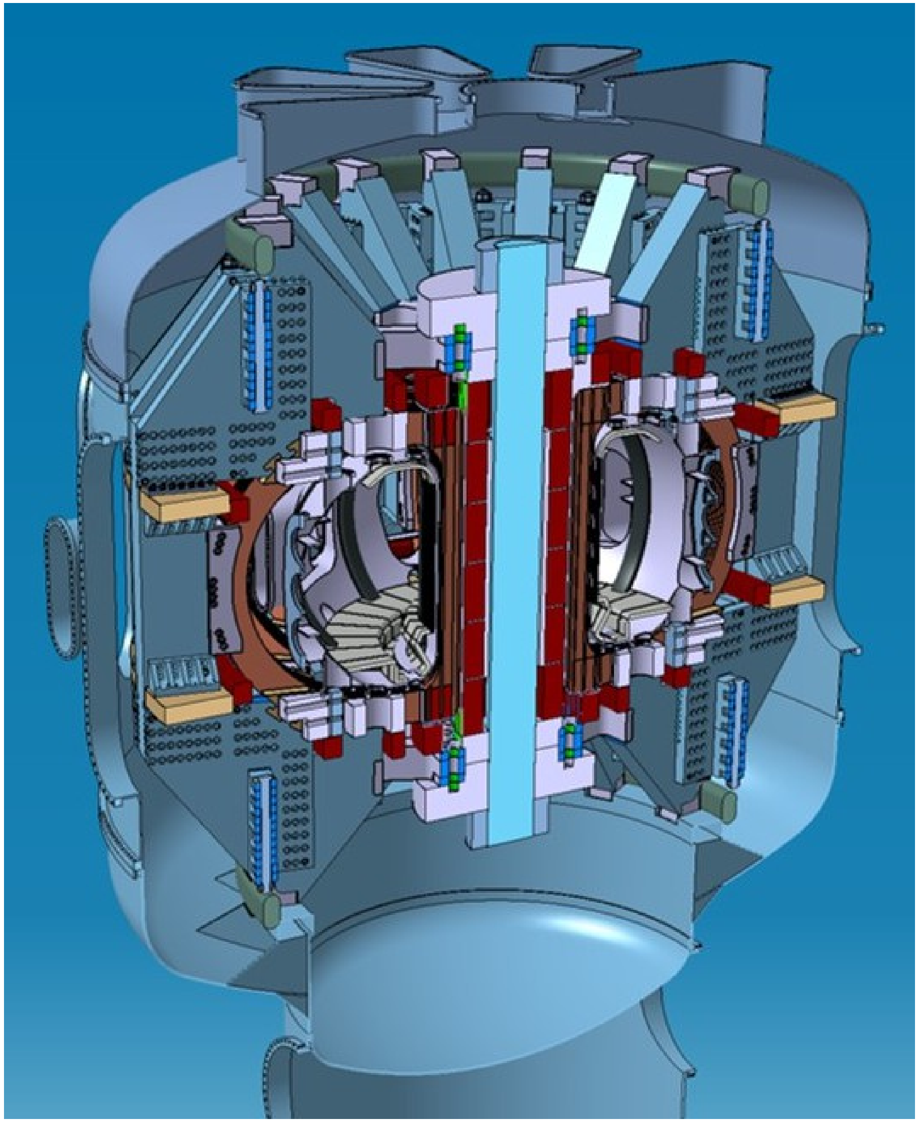
2. Simulations of plasmas during instabilites (ELMs), where $r_{Li} > L_{gap}$

- **Supercomputers like IT4I are very useful** when trying to achieve such simulations!

EXTRA SLIDES

COMPASS-U

- **1.5 times larger than COMPASS**
- Funding: **OP VVV project**, results should be known in **early 2018**
- **ITER** and **DEMO** relevant geometry
- **High magnetic field** (5 T), high density operation ($\sim 10^{20}$ m^{-3}), pre-cooled coppoer coils
- Advanced plasma configurations (double null, snow-flake)
- Closed and well diagnosed high density divertor
- **Hot-wall operation** (~ 300°C)
- **High power fluxes** in the divertor ($\lambda_q \sim 1$ mm)



Relevant publications

- **J.P. Gunn et al.**, *"Surface heat loads on the ITER divertor vertical targets"*, *Nucl. Fusion* **57** (2017) 046025
- **M. Komm et al.**, *"Particle-in-cell simulations of the plasma interaction with poloidal gaps in the ITER divertor outer vertical target"*, Nucl. Fusion **57** (2017) 126047
- **M. Komm et al.**, *"On thermionic emission from plasma-facing components in tokamak-relevant conditions"* **59** (2017) 094002
- **M. Komm et al.**, *"Simulations of thermionic suppression during tungsten transient melting experiments"*, accepted in Phys. Scripta (2017)
- **M. Komm et al.**, "Three-dimensional particle-in-cell simulations of gap crossings in castellated plasma-facing components in tokamaks", *Plasma Phys. Control. Fusion* **55** (2013) 025006
- **R. Dejarnac et al.**, *"Numerical evaluation of heat flux and surface temperature on a misaligned JET divertor W lamella during ELMs"*, Nucl. Fusion **54** (2014) 123011
- **R. Dejarnac et al.**, *"Effect of misaligned edges and magnetic field orientation on plasma deposition into gaps during ELMs on ITER"*, J. Nucl. Mat. **415** (2011) S977–S980
- **M. Komm et al.**, *"Particle-in-cell simulations of plasma interaction with shaped and unshaped gaps in TEXTOR"*, Plasma Phys. Control. Fusion **53** (2011) 115004
- **R. Dejarnac and J.P. Gunn**, "Kinetic calculation of plasma deposition in castellated tile gaps", J. Nucl. Mat. **363-365** (2007) 560-564

3D simulations of gap crossings

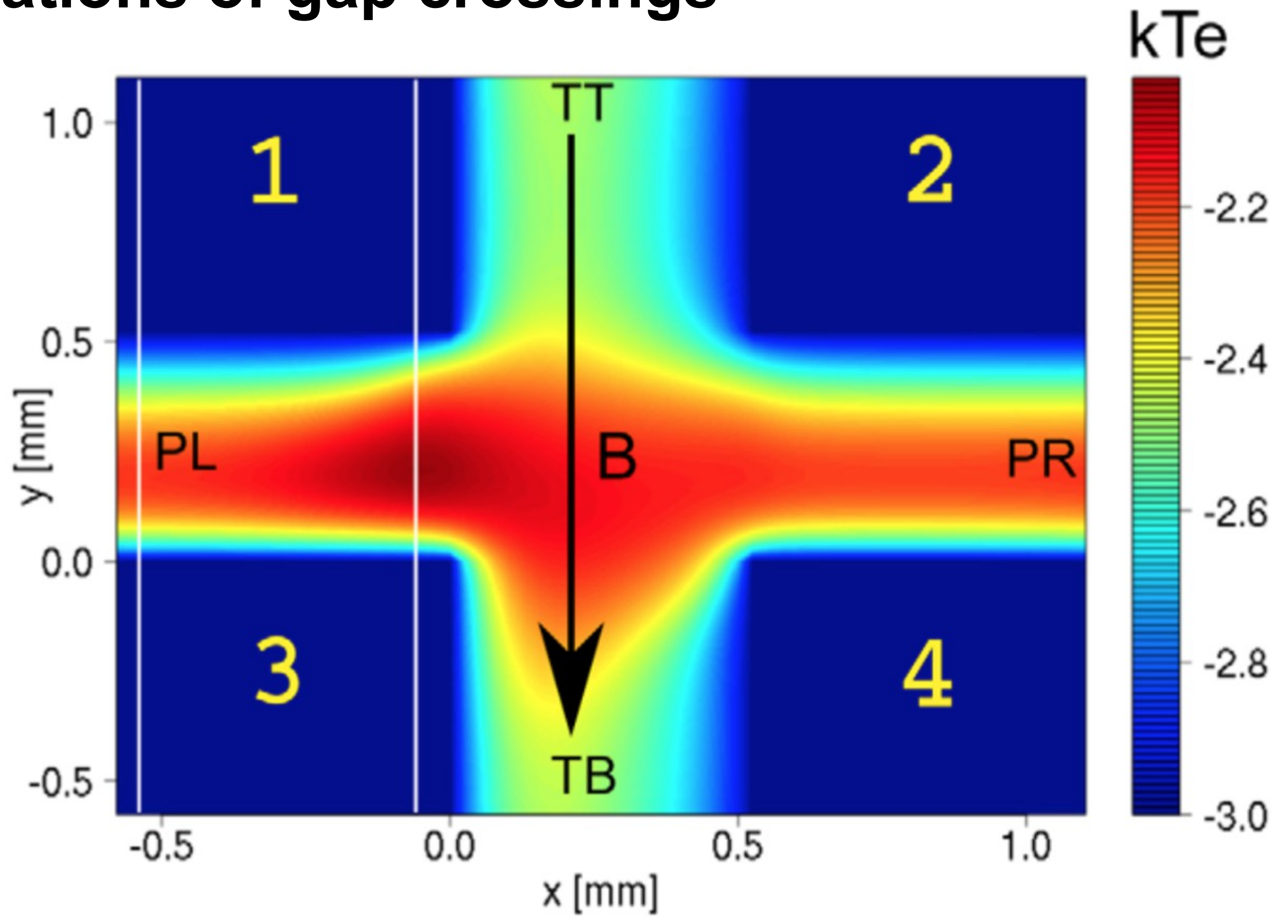
- 2D simulations allow to study poloidal and toroidal gaps separately

- What happens at the crossing between the gaps?

- Full 3D simulations required – SPICE3 was developped

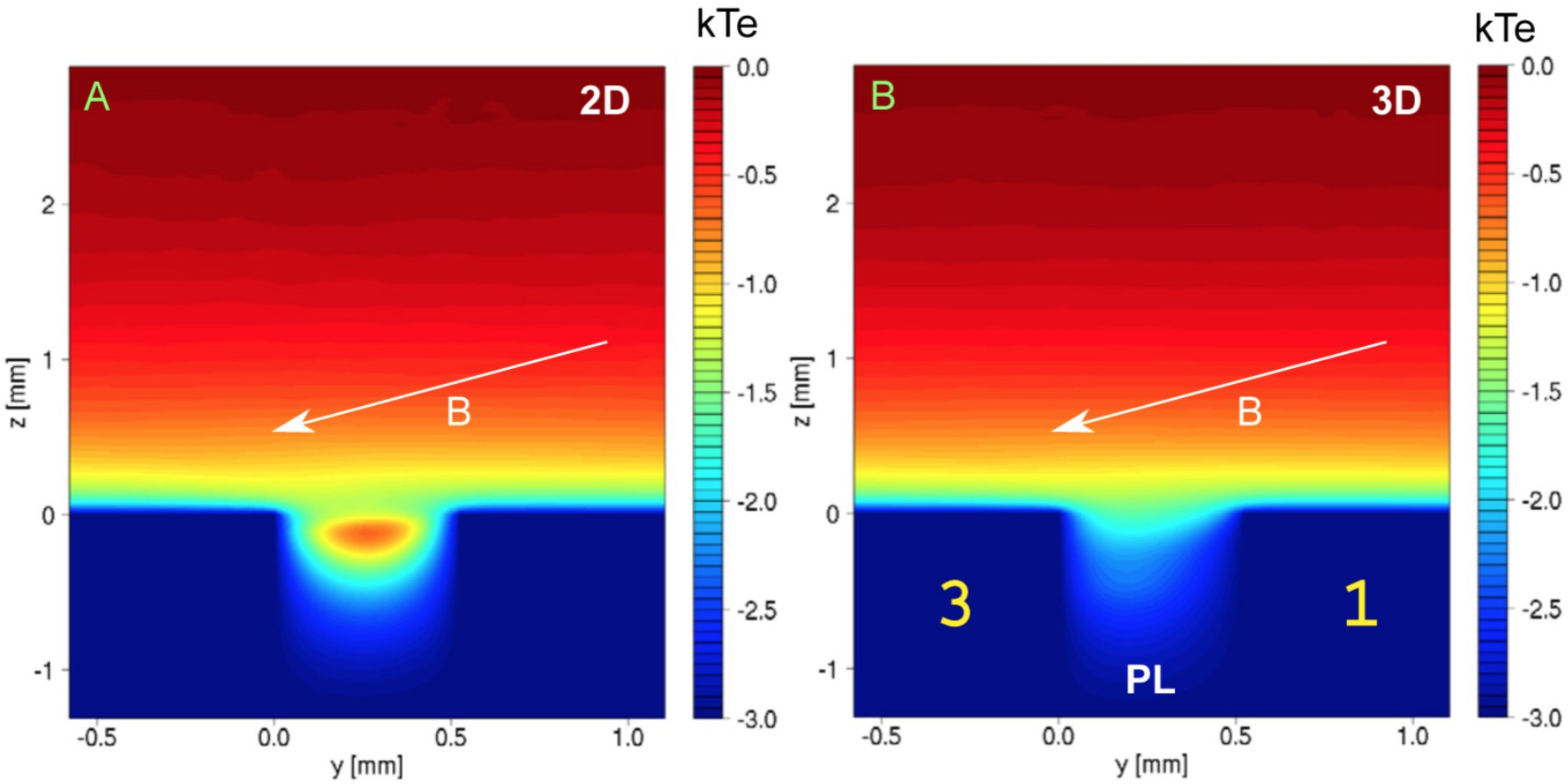
- Simulated conditions relevant to contemporary tokamaks (TEXTOR) $T_e = 25$ eV, $n_e = 2E18\ m^{-3}$, B = 2 T

- Published in: M. Komm et al. *Plasma Phys. Control. Fusion* **55** (2013) 025006



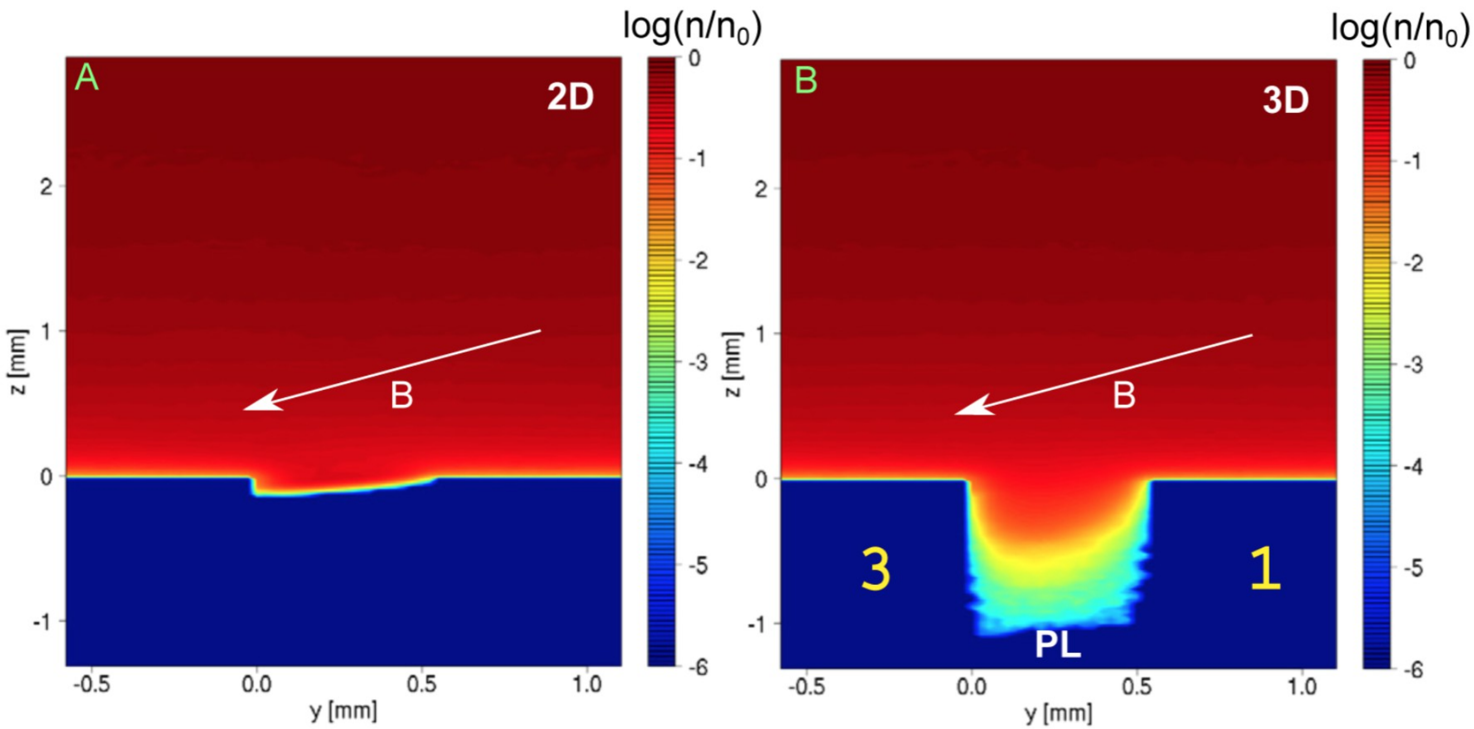
Top view of the gap crossings with potential profile

Surprise: the potential profile in poloidal gap is quite different!

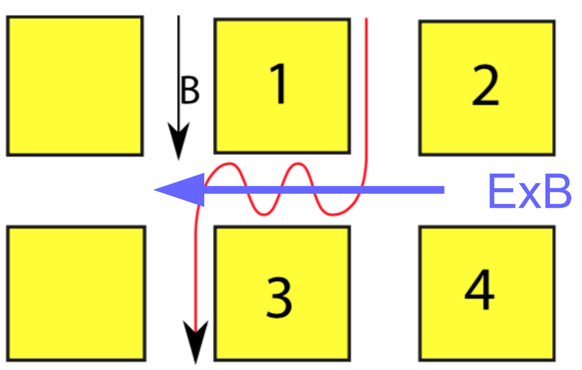


Potential structure is in some cases formed in magnetic shadow where only ions can reach – Electrons have too small Larmor radii

However in 3D the gap was full of electrons!



Reason: electrons can leak into poloidal gap via the crossing. The negative potential of the tiles does not allow them to reach the surface so they bounce and are dragged by the ExB drift throught the gap



Fortunately the potential structure does not appear in ITER-like scenarios – 2D PIC model is valid