Fully kinetic modelling of the tokamak Scrape-off Layer

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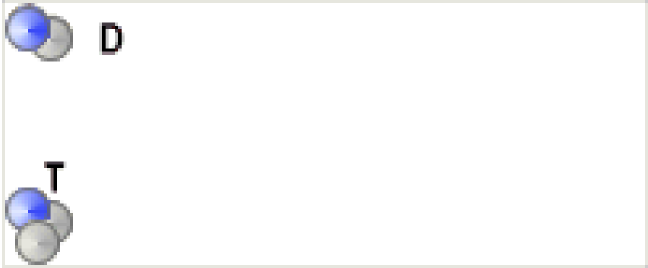
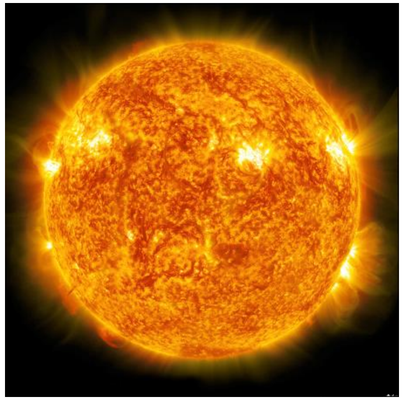
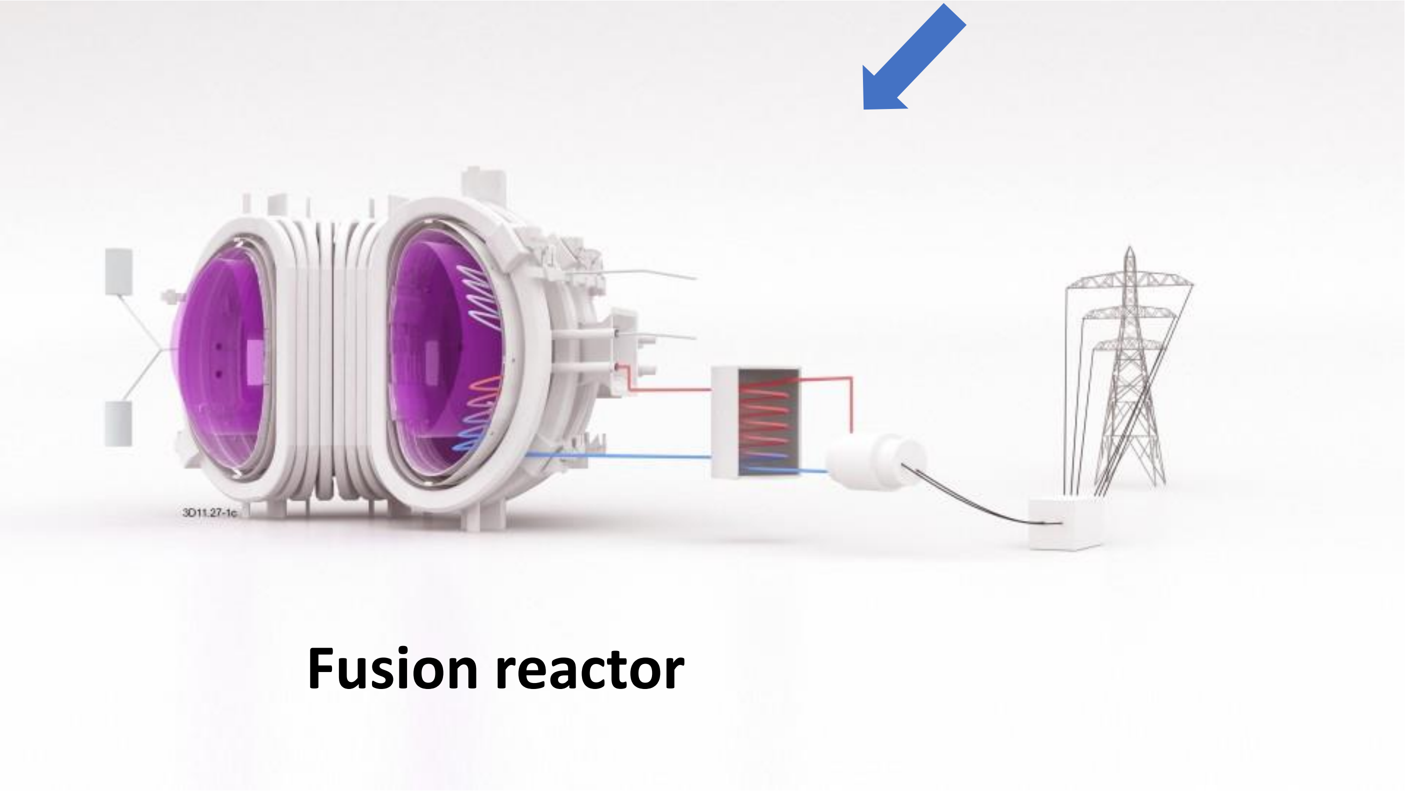
Motivation (nuclear fusion)



$D + T \rightarrow He + n + 17.6\ MeV$





Fusion reactor

Available fuel

D in water: $c_D \sim 0.0312\%$

$Li + n \rightarrow T + He$

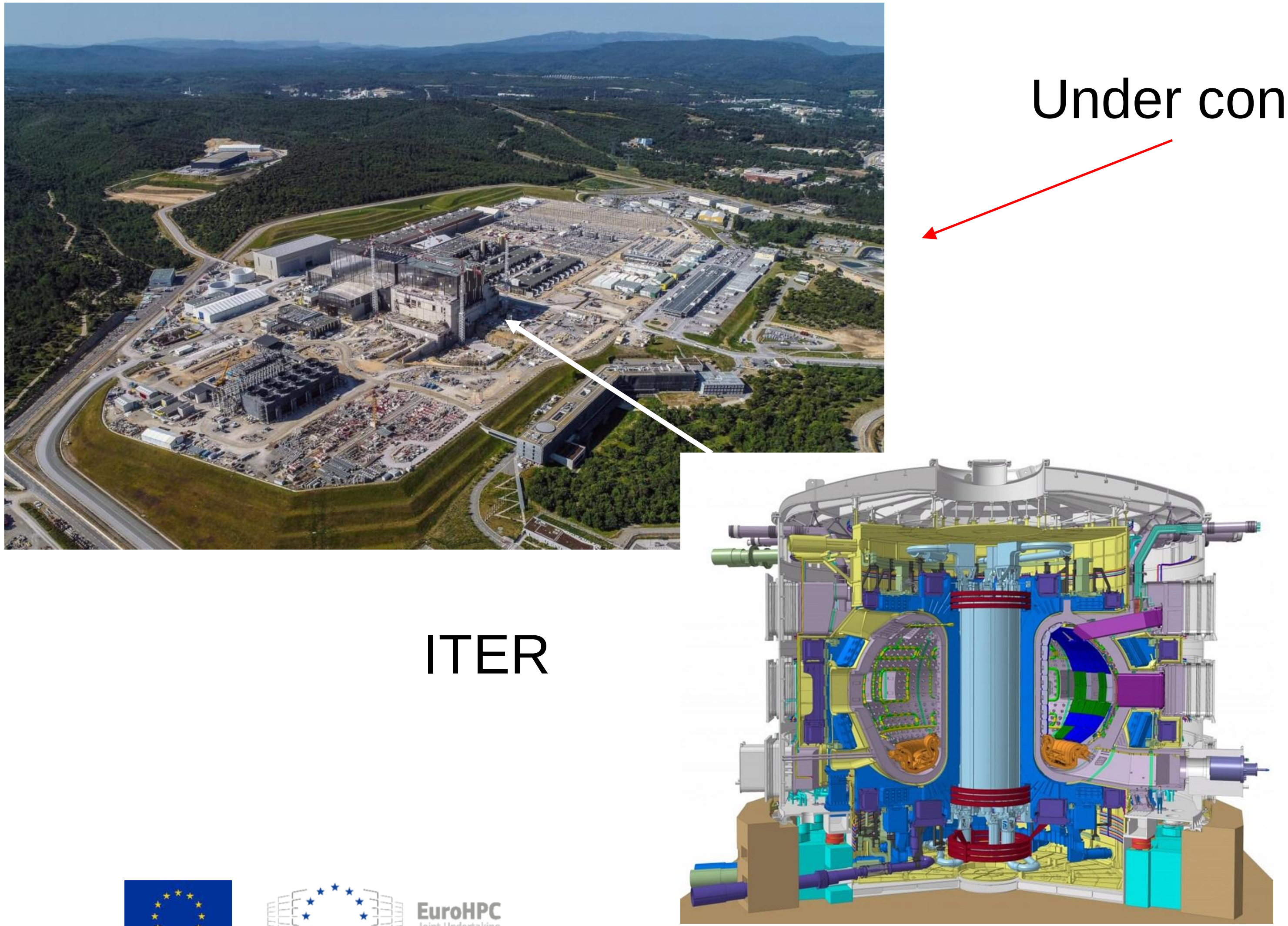
Li in the earth crust: $c_{Li} \sim 0.002\%$

Contains energy sufficient to satisfy energy demand of an average family for 1 year!

Test fusion facilities: tokamaks

Under construction

Under planning



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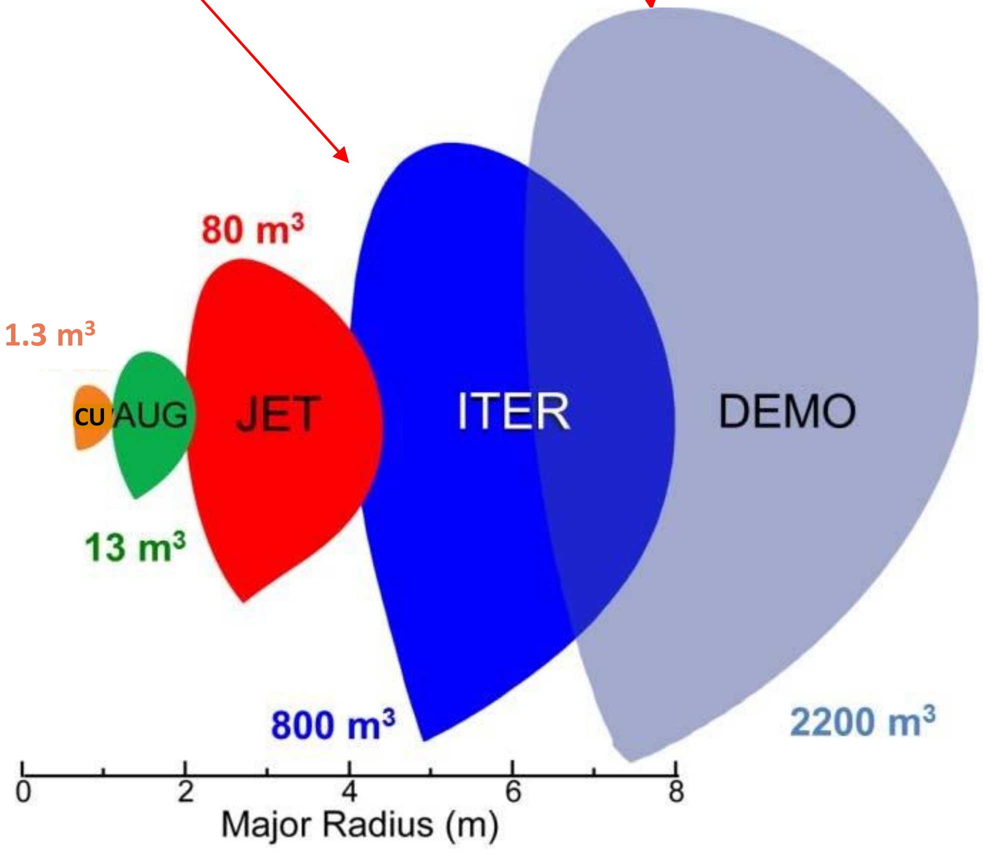
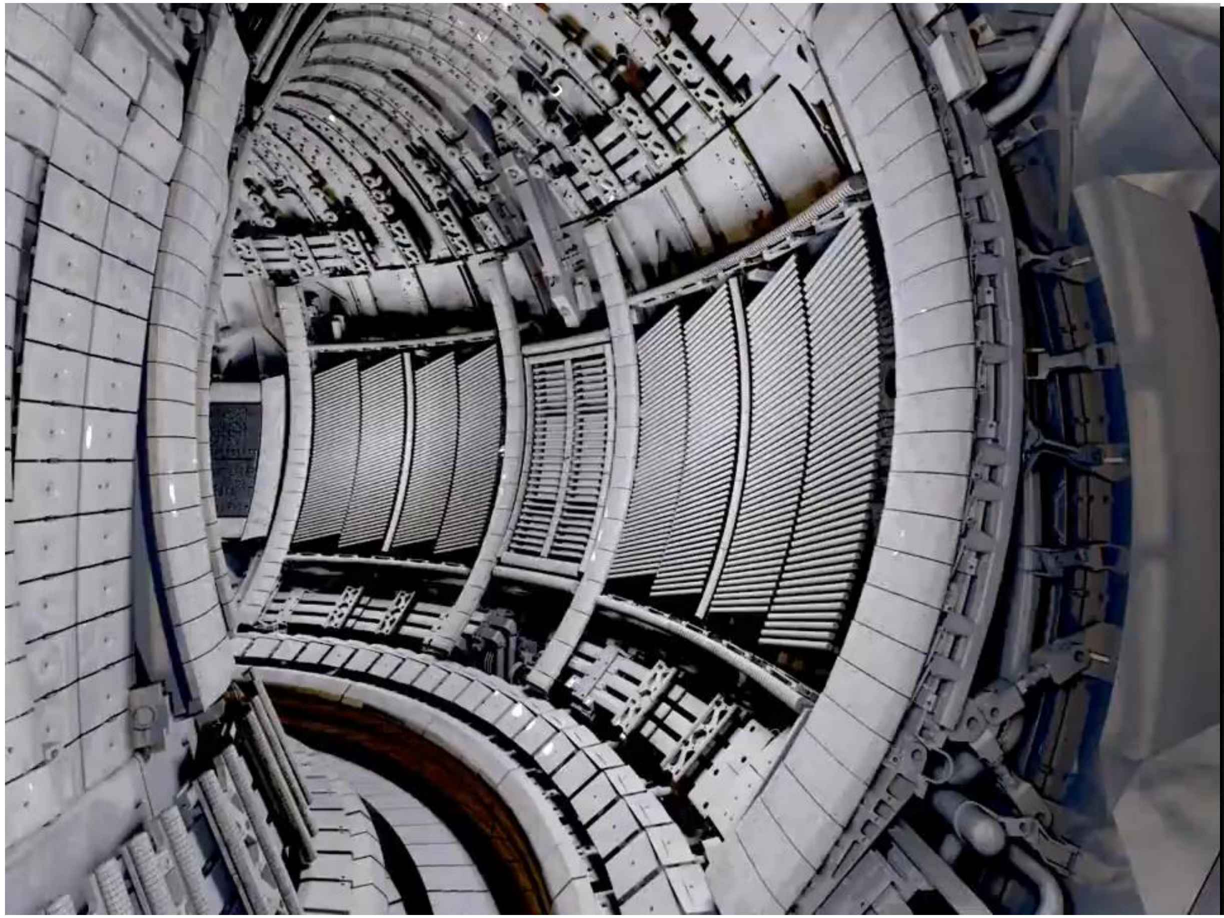
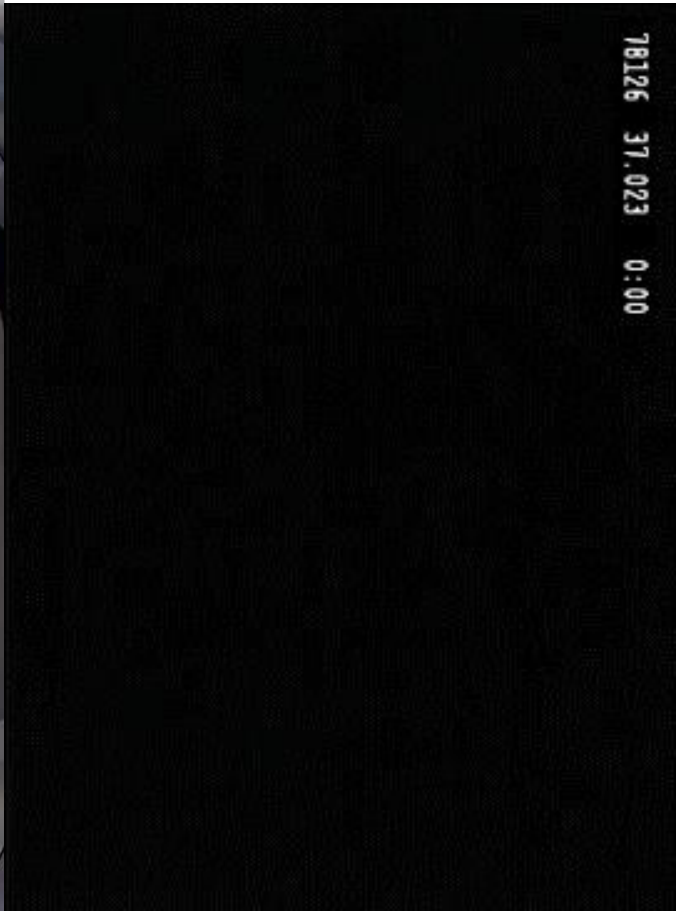


JET – Joint European Tokamak





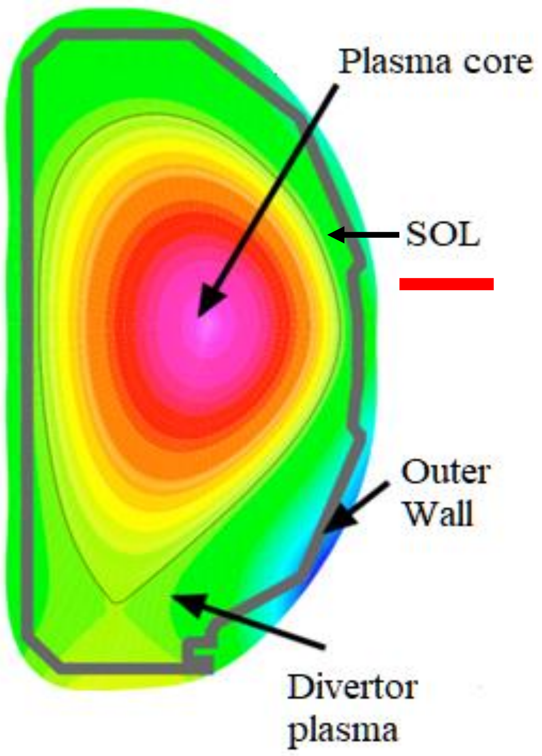
Temperature required for fusion > 100 000 000 C°

Plasma temperature at the wall ~ 100 000 C°

Inside JET chamber

Courtesy of EUROfusion: https://www.euro-fusion.org

The main challenges of the SOL kinetic modelling



Temperature
0.5 eV – 5 keV

Resolution in velocity space:

$$0.01V_T \leq V \leq 30V_T$$

Space
1 µm – 20 m

Resolution in space:

$$dx \leq 5\times10^{-7}\ m \qquad N_{dx} > 10^6$$

Time
0.1 ps – 1 ms

Resolution in time:

$$dt \sim 10^{-13}\ s \qquad N_{dt} > 10^9$$

SOL (Scrape-Off Layer)

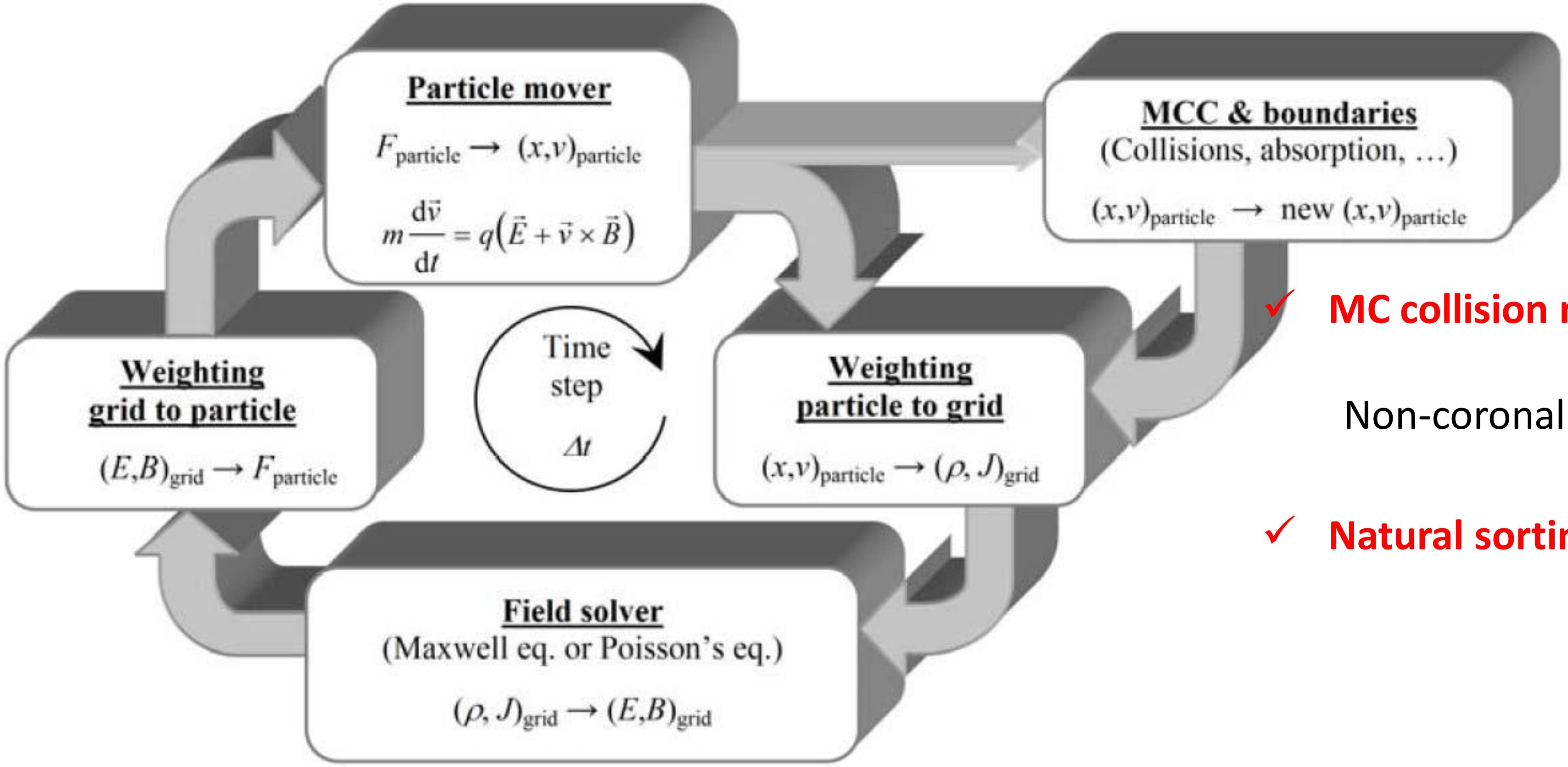
- Plasma exhaust
- Impurity content
- Tritium retention
- **Kinetic effects are essential**

PLASMA PEPSC

The structure of the BITx, x=1,3 codes

1D3V (BIT1) and 3D3V (BIT3) electrostatic PIC + Monte Carlo

Originated from **XPDP1** code
from Berkeley University



Particle mover

$F_{\text{particle}} \rightarrow (x,v)_{\text{particle}}$

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

MCC & boundaries
(Collisions, absorption, …)

$(x,v)_{\text{particle}} \rightarrow \text{new } (x,v)_{\text{particle}}$

Weighting grid to particle

$(E,B)_{\text{grid}} \rightarrow F_{\text{particle}}$

Time step Δt

Weighting particle to grid

$(x,v)_{\text{particle}} \rightarrow (\rho, J)_{\text{grid}}$

Field solver
(Maxwell eq. or Poisson's eq.)

$(\rho, J)_{\text{grid}} \rightarrow (E,B)_{\text{grid}}$

- ✓ **MC collision model**

  fast, no limits on collision types[2]

  Non-coronal approximation for high density plasmas[3]

- ✓ **Natural sorting, cell-based particle indexing**

  Optimal use of the cache hit

  easy space decomposition

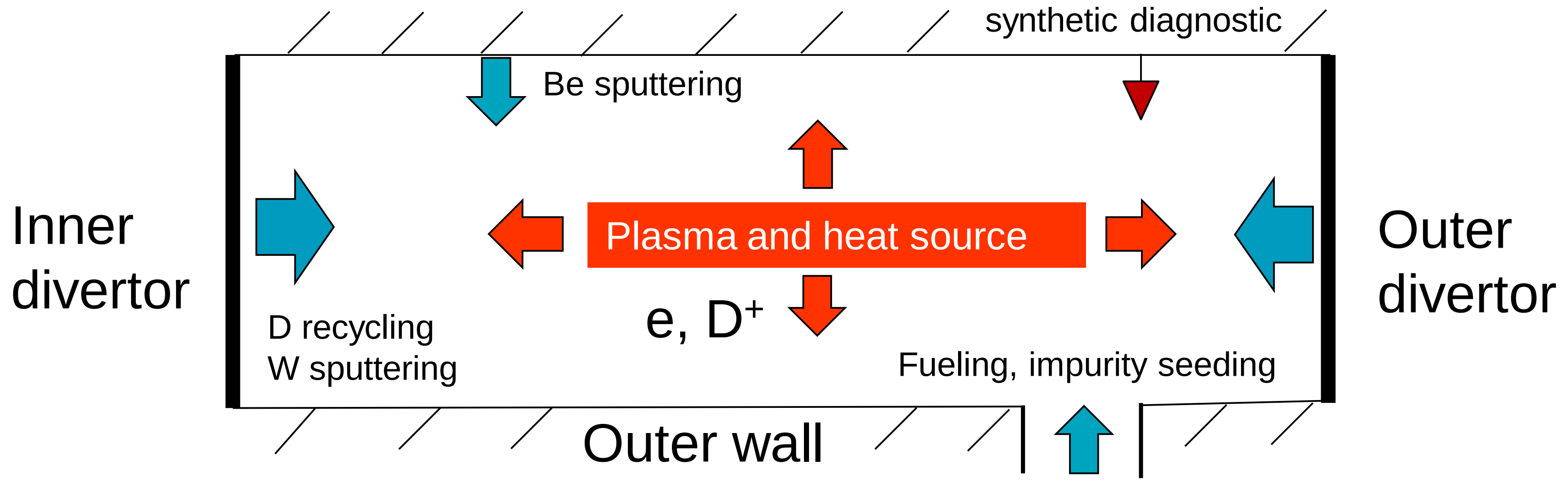
  no limitation of the system size[4]

- ✓ **BIT1 - Physics based Poisson solver**

accurate, fast and highly scallable[1]

[1] D. Tskhakaya, et al., 18th Euromicro Conference proceedings (2010)
*[2] D. Tskhakaya, et al., Contr. Plasma Phys., **48** (2008)*
[3] D. Tskhakaya, Eur. J. Phys. D., online (2023)
*[4] D. Tskhakaya, et al., J. of Comp. Phys., **225** (2007)*

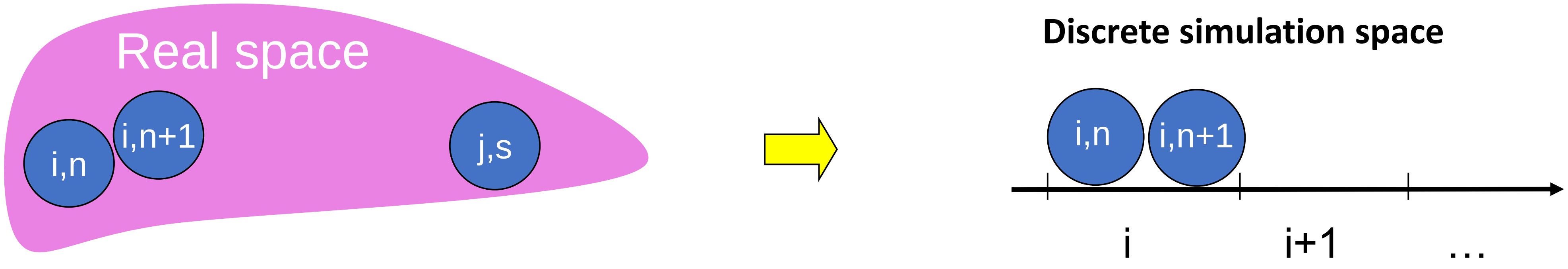
The geometry of BIT1,3 simulations



- Particle, momentum and energy conserving nonlinear operators for elastic and inelastic collisions
- Sophisticated Plasma-Wall interaction module
- Plasma and impurity injection ports
- Synthetic diagnostics (Langmuir Probe, Spectroscopy)
- All possible diagnostics: plasma and field profiles, angular, velocity and energy DFs at any location at any time.

Natural sorting

Particles curry the cell index, e.g. the coordinate of the particle *n* is saved as $x[i][n]$



- ✓ Neighboring particles in a real space are neighbors in the computer memory: cache-hit increases
- ✓ Cells are statistically independent: all collision probabilities are calculated separately. Easy to find collision partners.
- ✓ Massive parallelization is straightforward: easy to identify particles crossing boundary of the core and have to be passed to the next core
- ✓ Particle trajectories are calculated with the same accuracy at each point

On accuracy of particle trajectory calculation in a large system

Large system with a fine resolution: $L >> \Delta x > |V\Delta t|$

Classical model

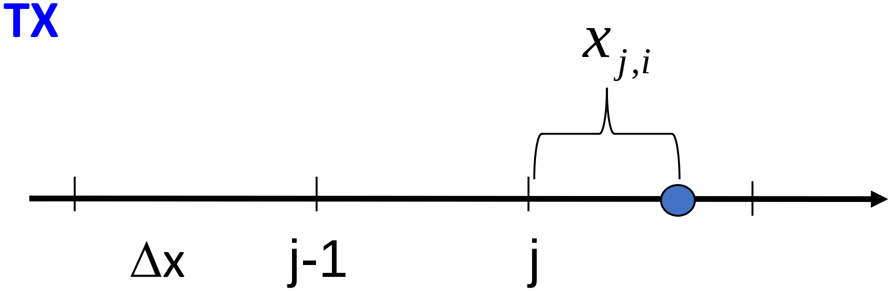
$x \sim 10\,m,\;\; V \sim 10^{4}\;\, m/s,\;\; \Delta t \sim 10^{-13}\, s$

$x_{i,t+\Delta t} = x_{i,t} + V_i \Delta t$ at the far end $x_{i,t} >> |V_i \Delta t|$

$$\frac{V\Delta t}{x} \sim 10^{-10}$$

Calculation accuracy decreases!

BITX



$$x_{actual,t} = j\Delta x + x_{j,i,t}$$

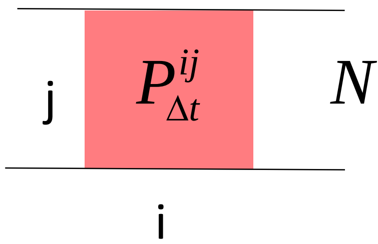
$$x_{j,i,t+\Delta t} = x_{j,i,t} + V_{i.x}\Delta t\,, \qquad x_{j,i,t} < \Delta x \sim V_{i,x}\Delta t\,,$$

Particle trajectories are calculated with the same accuracy at each point → no near/far end asymmetry

Collision operators in the BIT1/3

i. Decision on collision

Non-counter based model



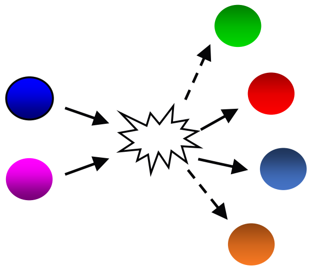
$$N_{\Delta t} = P^{ij}_{\Delta t} N_{ij}$$

Scales as ~$\boldsymbol{N}_{\mathbf{cell}}$

if yes

ii. Calculation of after-collision velocities

Binary collision model



particle number, energy and momentum are **conserved**

Collision types[2]

- 2 → 2 - elastic, excitation, charge-exchange,…
- 2 → 1 - recombination (radiative)
- 2 → 3 - dissociation, ionization
- 2 → 4 - double ionization, dissociative ionization
- 3 → 2 - recombination (three-body)

Implemented elements

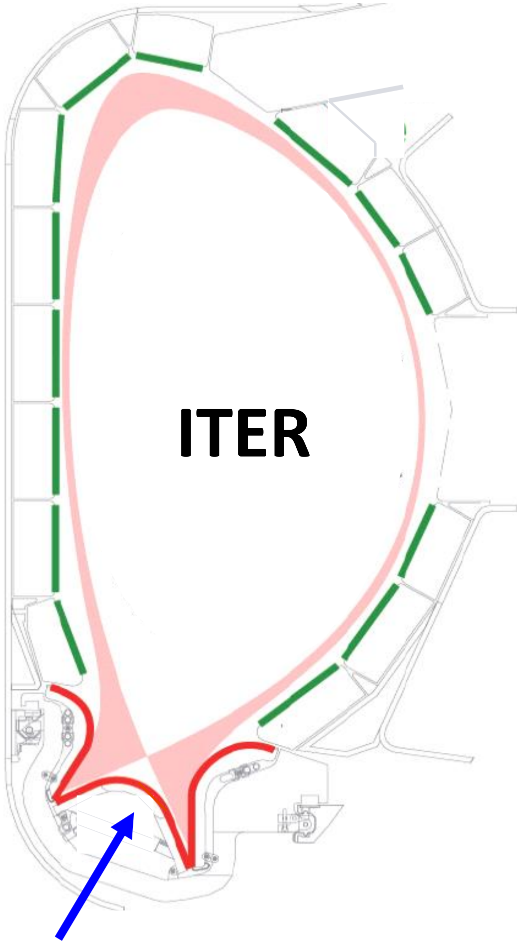
H(H/D/T), H_2, He, Li, C, Be, Ne, Ar, O_2, W

$$\sigma(E,T,n) = \sigma(E)\frac{R(T,n)}{R_{n=0}(T)}$$

From collisional-radiative model

Non-coronal effects implemented via DCSM (Dressed Cross-Section Model)

Simulation example[5]



Divertor plates. The limit of acceptable power load – 10 MW/m^2.

Estimatimated power loads to the ITER divertor from the different BIT1 simulations

Run	q_e [MW/m^2] ID / OD	q_i [MW/m^2] ID / OD
Original, Ne$^{+i<2}$	3.7 / **15.7**	2.2 / 3.8
Model with Ne$^{+i<5}$	7.2 / **13.2**	3.1 / 4.7
DCSM ion. D, Ne$^{+i<5}$	**0.9** / **0.9**	2.7 / 3.1
DCSM ion. D/Ne, Ne$^{+i<7}$	**0.8 / 0.8**	2.4 / 2.8
DCSM ion./rec D/Ne, Ne$^{+i<7}$	**0.7 / 0.8**	2.3 / 2.7

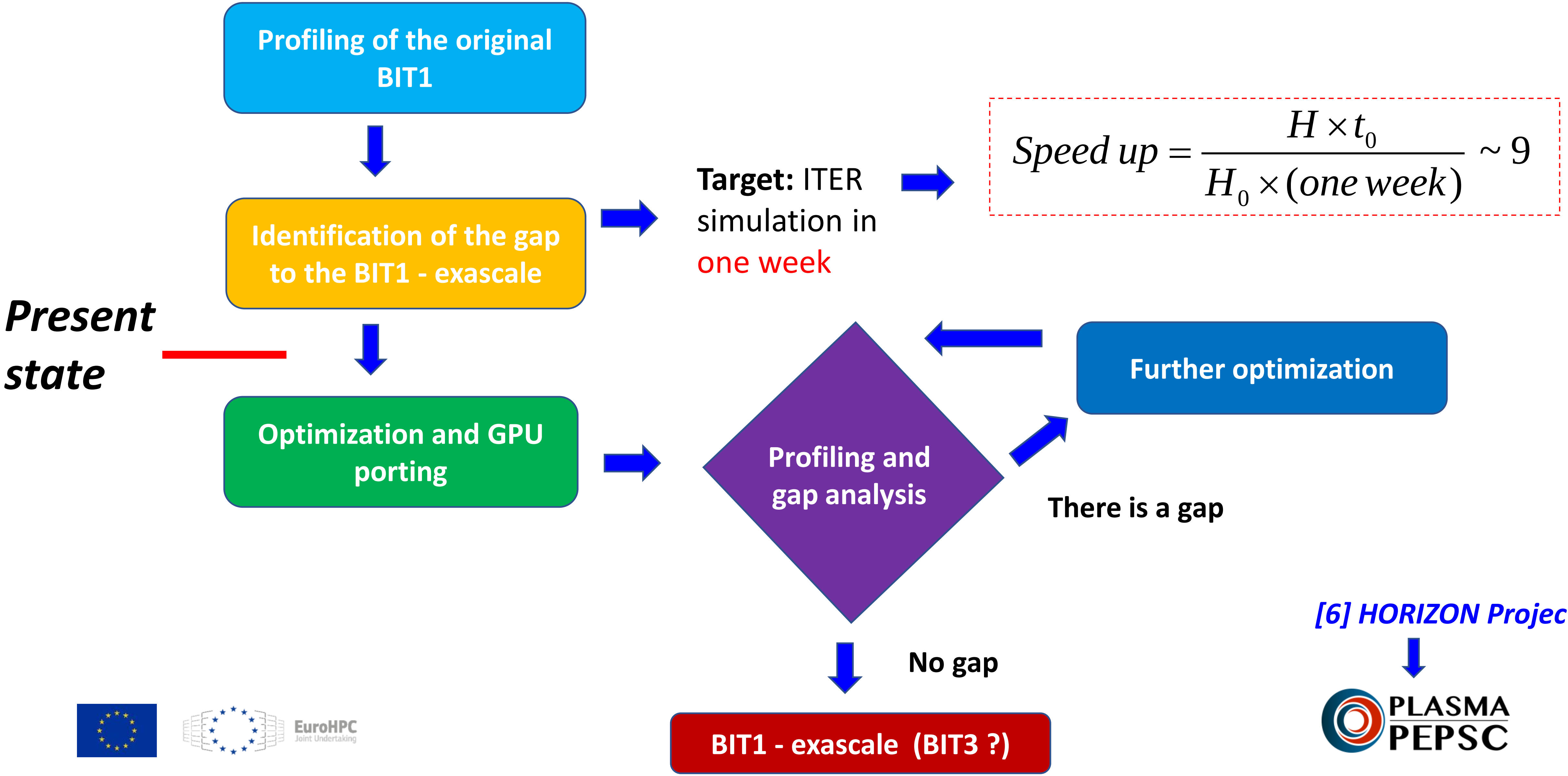
Each step required **10 – 100 M core hours!**

10 core hours ~ 20 days (on Marconi / IFERC)

Exascale modelling

[5] D. Tskhakaya, ITER Scientist Fellows' Network, June 2023

BIT1 exascaling workflow[6]



Profiling of the original BIT1

Identification of the gap to the BIT1 - exascale

Target: ITER simulation in one week

$$Speed\ up = \frac{H \times t_0}{H_0 \times (one\ week)} \sim 9$$

Present state

Optimization and GPU porting

Profiling and gap analysis

Further optimization

There is a gap

No gap

BIT1 - exascale (BIT3 ?)

[6] HORIZON Project

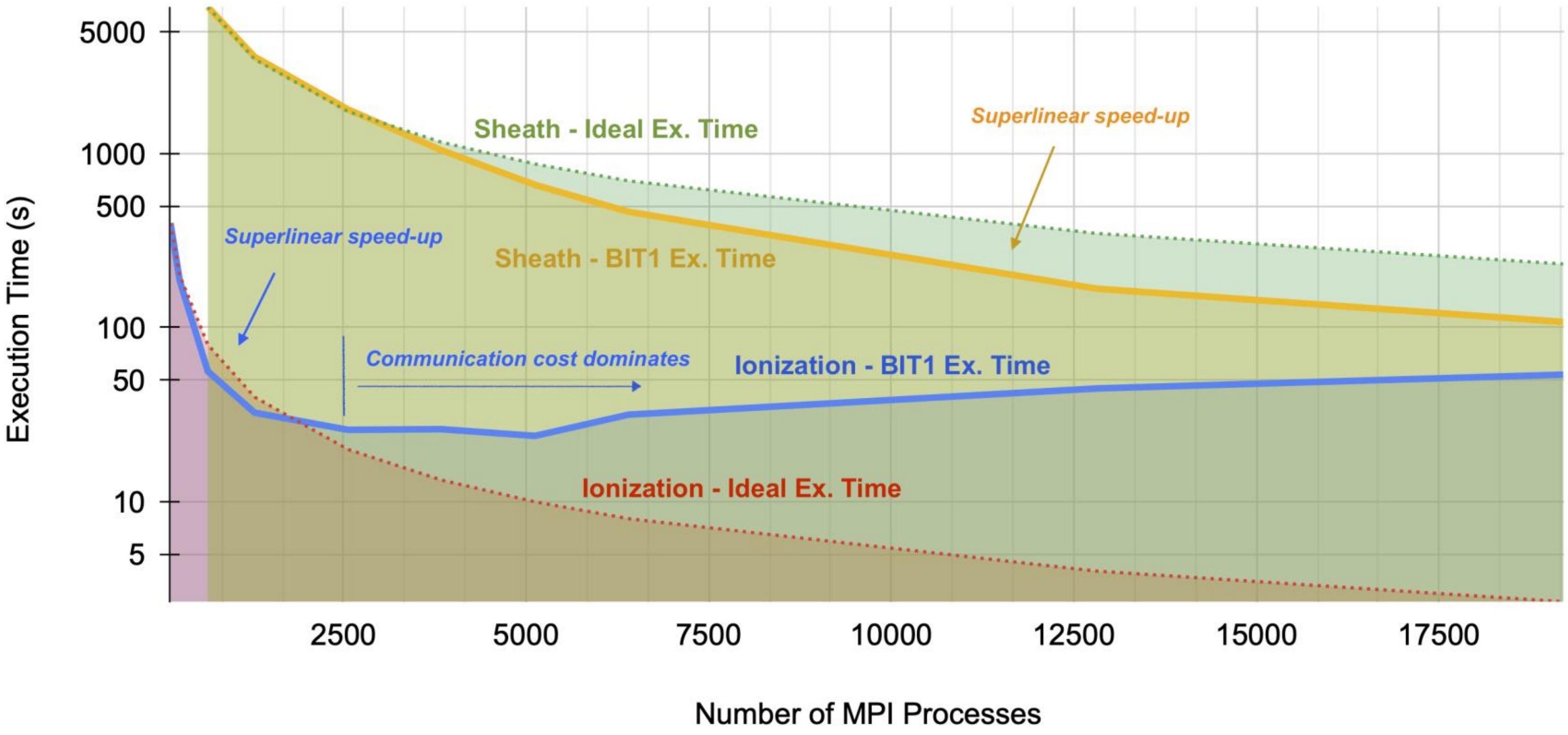
PLASMA PEPSC

EuroHPC Joint Undertaking

Main results of the BIT1 profiling[7]

Two case have been considered

- *Small system used for plasma ionization tests – "Ionization"*
- *Heavy production run – "Sheath"*



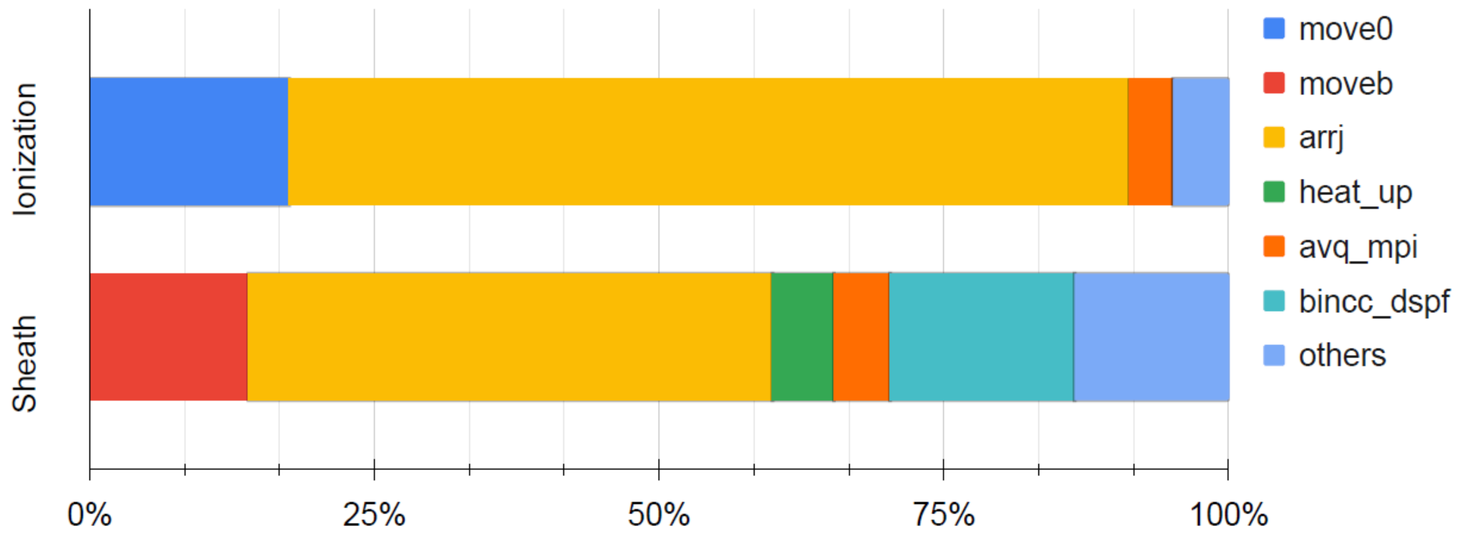
Strong scaling test on Dardel supercomputer

- ***The BIT1 shows hyper-scaling;*** *for a heavy production run > 17 500 cores*
- *The BIT1 performance depends on the problem size and* ***effective LLC usage****.*
- *The serial BIT1 is a* ***highly memory-bound*** *code.*

Data are in [%]	Baseline Size	10% Reduced size	20% Reduced size	Cache test
L1 Load Misses	3.43	2.51	2.17	5.53
LLC Load Misses	99.07	52.25	47.51	18.95

[7] J. Williams, et all., submitted for publication

Percentage breakdown of the BIT1 functions



moveb() - **particle pusher**

Leap-Frog scheme, adjusts solver to the given magnetic field configuration,

no rank communication is required (highly optimized)

bincc_dspf() – **Binary collision operator**

no rank communication is required (highly optimized)

arrj() – **arranjing particles** into proper cells and ranks

no rank communication is required; **at present** we are trying to **optimize it**

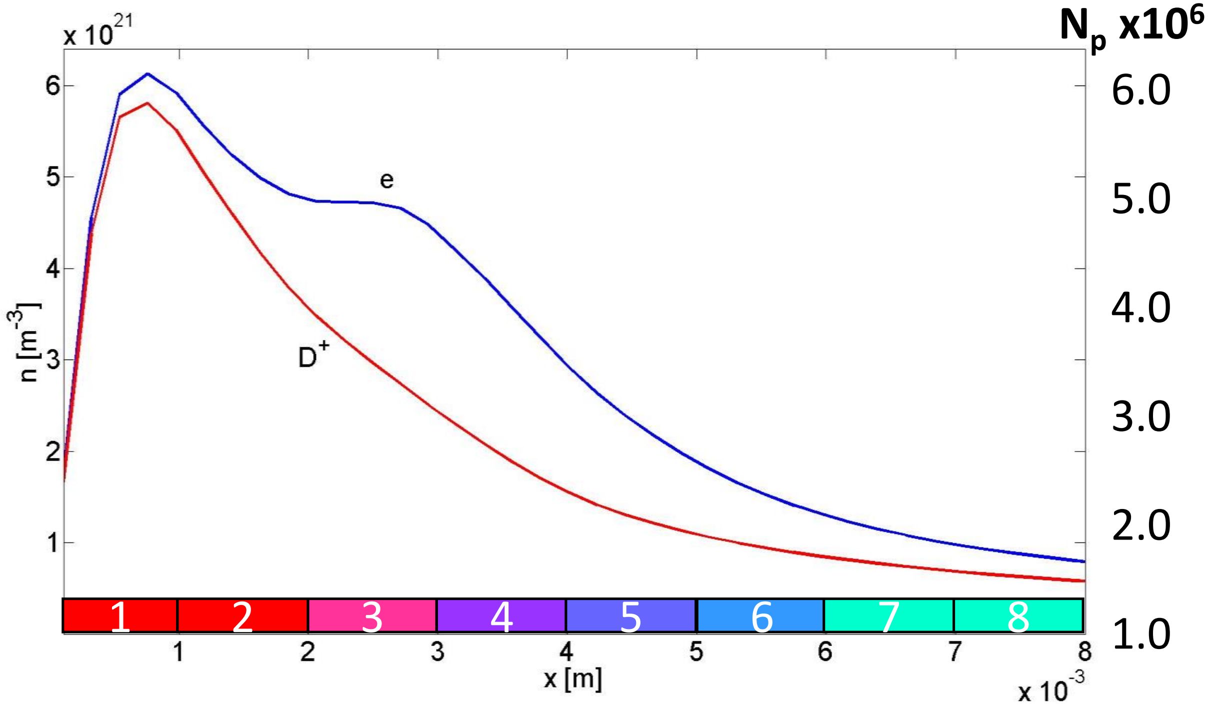
Optimization strategies: nonuniform dynamic space decomposition

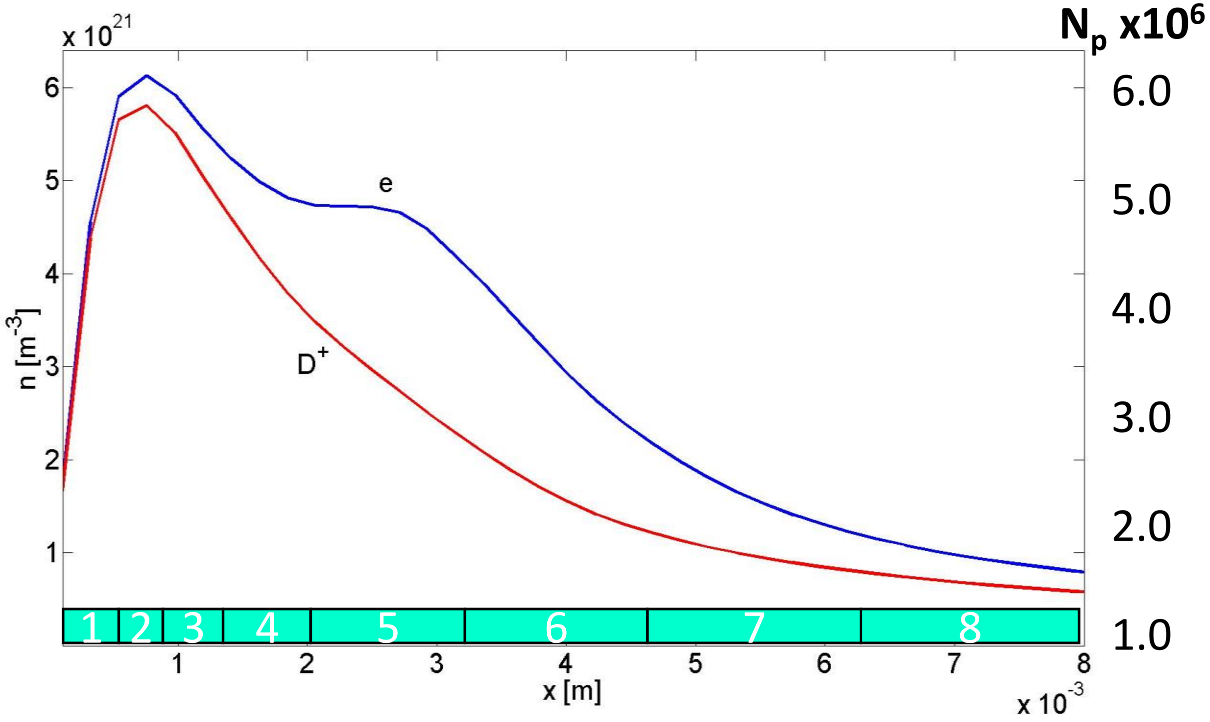
The present versions of BIT1,3 use a fixed **uniform space decomposition**

- **Advantage** – simple, universal implementation
- **Disadvantage** - the simulation speed is defined by the cores with the **highest particle number**, i.e. plasma density

Nonuniform dynamic space decomposition

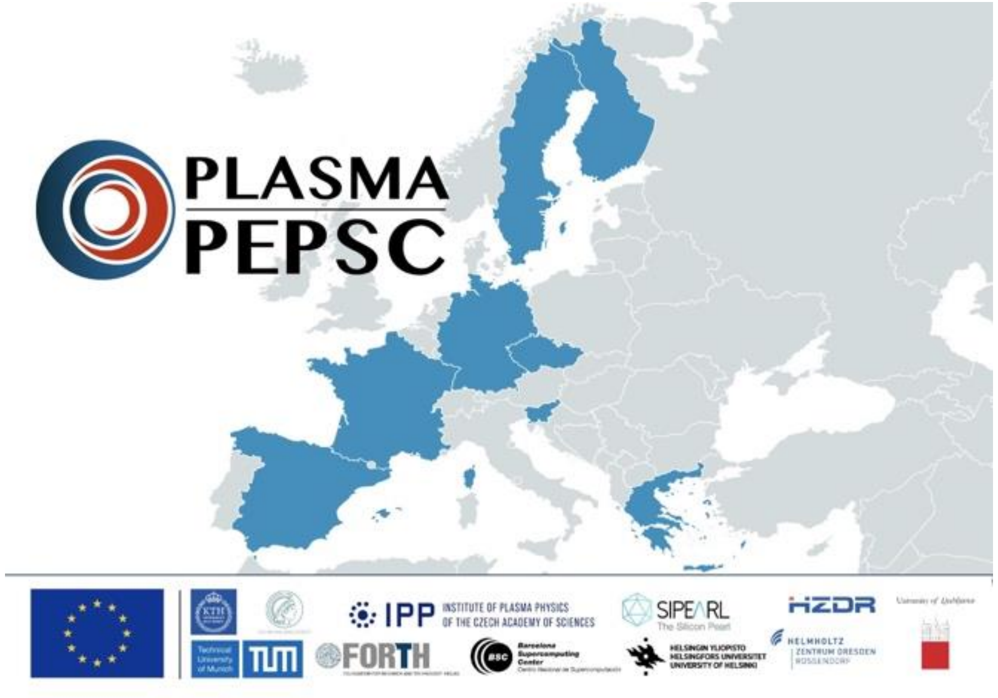
- **Advantage** – uniform core load, high scaling
- **Disadvantage** – complex implementation, not universal, requires **significant code updates**





Summary

- For designing and performance optimization of next generation fusion test facilities kinetic modelling of the plasma edge is required. The corresponding full scale simulations can only be performed on the **exascale platform**. The **BIT1** and **BIT3** codes are the candidates of such porting .
- „Exascalization“ of the BIT1 is started under the HORIZON **Plasma-PEPSC** (2023 – 2027).
- The first profiling tests indicate that the BIT1 exhibits **hyper-scaling** for large simulations for up to at least **18 000 cores**. A high **memory-bound** seem to be the reason of such behavior.
- Gap analysis indicated, that for reaching the desired exascale performance **9 times** increase of the simulation speed is required.
- At present, we are **optimizing „slow“ functions**, such as arrj() – responsible for particle sorting and plan to introduce **nonuniform dynamic space decomposition** in to the code.



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