On the role of integrated computer modelling in fusion technology

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Outline and Background

- Computer modelling plays an increasingly important role in fusion design and technology:
  - complexity of the physical processes involved (plasma, materials, engineering)
  - highly interconnected nature of systems and components (“system of systems”)

call for support from sophisticated and integrated computer simulation tools.

- This presentation reviews the state-of-the-art of (coupled) computer modelling of use for reactor design (focus on breeding blanket and integrated 1st wall) in terms of
  - Neutronics
  - Materials behaviour (including plasma-materials interaction, radiation effects and compatibility with fluids)
  - Magnetohydrodynamics thermofluid issues and thermo-hydraulic aspects
  - Simulations of plasma transport out of the confinement region to determine heat and particle loads on plasma facing components

The authors gathered together around the idea of writing such a review

The presenter is only expert in one of the fields

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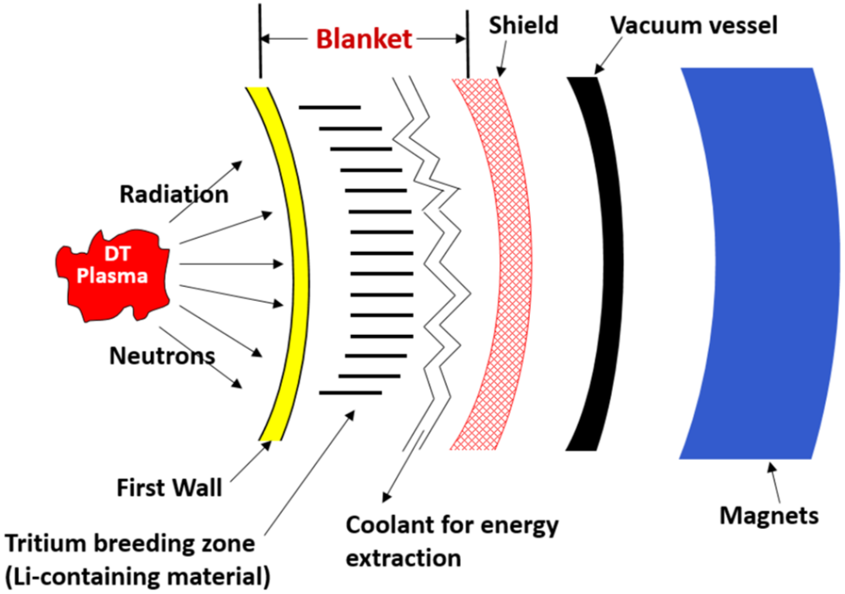
Focus on the breeding blanket

The blanket/FW is an in-vessel component located between vacuum vessel and plasma.

Its main purpose is threefold:



1) **To assure self-sufficiency of the fusion reactor with regard to tritium** (by producing, from lithium, at least the same amount of tritium as consumed in the plasma)

2) **To convert fusion energy into heat** (to produce electricity by using a turbine-driven generator)

3) **To act as a radiation barrier** (such that the components behind the breeding blanket receive the lowest possible amount of radiation)

No Breeding Blanket has ever been built or tested → crucial role of computer modelling!

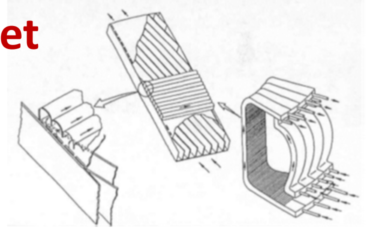
Many different choices can be made for the blankets, leading to plenty of designs

- **Breeder**: ***LM*** (Li, PbLi), ***SB*** (Li_2O, $LiAlO_2$, Li_2ZrO_3, Li_4SiO_4), ***MS*** (FLiBe, FLiNaBe)
- **Cooling strategy**: *self-cooled, separately-cooled, dual-coolant*
- **Coolant**: *LM, He, water*
- **Use of neutron multiplier**: *Be, Pb*
- **Use of qualified or "new" materials**
- **Flow orientation** (for LM or MS blankets): *toroidal, poloidal, radial*
- **Location:** *Inboard, outboard*
- **Maintenance scheme**: *vertical, radial*
- **Configuration**: *"banana", module* (~2 m)
- …

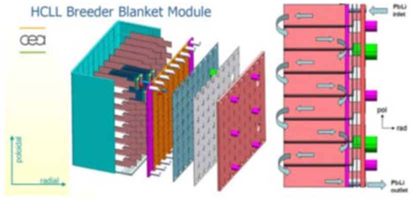
There is no “back up”… All blankets have their issues

- **Self-cooled LM blanket**
  - highest rank by BCSS
  - low crack tolerance
- **Separately cooled LM blanket**
  - available structural materials and fabrication technologies
  - T permeation from PbLi into He is a serious safety issue
- **Dual-coolant LM blanket**
  - high thermal efficiency (>40%)
  - relies on still underqualified SiC FCI
- **Molten salt blanket**
  - low MHD pressure drop
  - low TBR and many chemistry issues
- **Solid breeder blanket**
  - robust design
  - pebble bed thermomechanics, low thermal efficiency

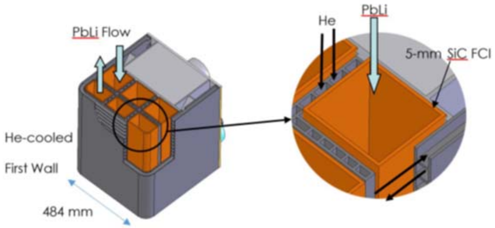
US self-cooled Li/Va blanket



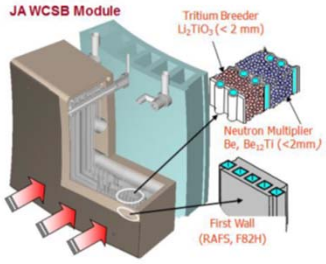
EU HCLL/WCLL blankets



US DCLL blanket (also EU)



JA water-cooled SB blanket
EU HCPB blanket



Integrated modelling for fusion neutronics

- Neutron irradiation causes activation of the structural materials up to the bioshield, with wide distribution of the radioactive sources, including activation of cooling water.
- **Neutronics specifics & challenges of large fusion tokamaks and stellarators :**
  - **Complicated 3D geometry** of substantially heterogeneous CAD models
  - **Large volumes** of 14 MeV neutron sources in D-T plasma
    - Monte Carlo (MC) method of radiation transport is most suitable for such complex geometry, especially for geometries with channels and gaps which open radiation streaming pathways
    - Use of **CAD-to-MC geometry conversion** is an inevitable part of the neutronics modelling process
    - Decay **gamma transport must be taken into account** for Shut-Down Dose Rate (SDDR) calculations – challenge to combine neutron transport and activation
- **Two integrated modelling approaches have been developed, T1 and T2:**
  - **Type T1** is **CAD-to-MC geometry conversion** modeling which allows the most accurate reproduction of the actual design and closest correspondence to reality to be achieved
  - **Type T2** is the methodology of **Shut Down Dose Rate** calculations including transport of decay gammas from distributed gamma sources

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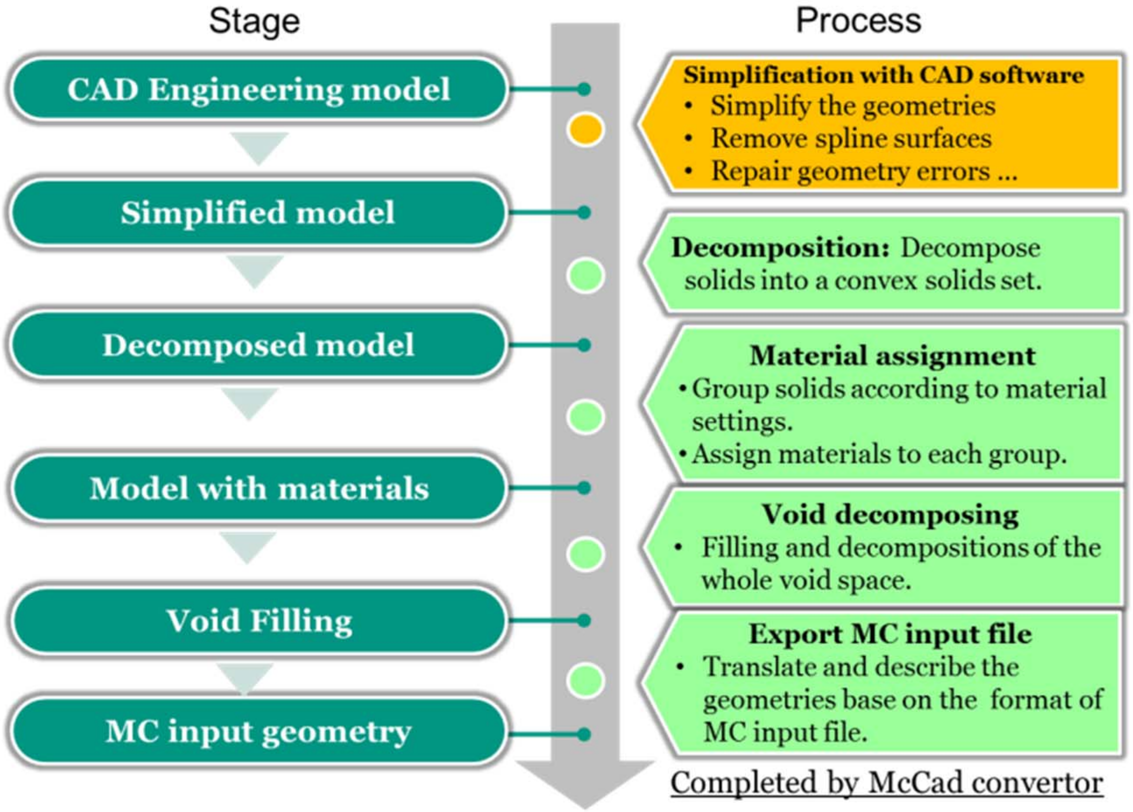
T1 integrated modeling: CAD-to-MC geometry conversion illustrated on the McCad modeling approach

Stages and processes of the CAD-to-MC model conversion with the McCad software [Ref. 1, 2]
McCad is available freely on github: https://github.com/McCadKIT/FreeCAD-McCad



Stage	Process
CAD Engineering model	
	Simplification with CAD software • Simplify the geometries • Remove spline surfaces • Repair geometry errors ...
Simplified model	
	Decomposition: Decompose solids into a convex solids set.
Decomposed model	
	Material assignment • Group solids according to material settings. • Assign materials to each group.
Model with materials	
	Void decomposing • Filling and decompositions of the whole void space.
Void Filling	
	Export MC input file • Translate and describe the geometries base on the format of MC input file.
MC input geometry	

Completed by McCad convertor

T1 using the MC model is suitable and sufficient for the following calculations:

- **neutron and photon fluxes**
- **nuclear heating (neutron and secondary photons)**
- **neutron damage (dpa)**
- **helium and hydrogen gas production**

[Ref. 1] D.Grosse et al., Status of the McCad geometry conversion tool and related visualization capabilities for 3D fusion neutronics calculations, Fusion Eng. Des. 88 (2013) 2210-2214.

[Ref. 2] L. Lu et al., Development of McCad as an Integrated Interface Tool for the CAD to MC Geometry Conversion, M&C 2017, Jeju, Korea, April 16-20, 2017.

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T2 integrated modeling: Rigorous 2-Step mesh-based (R2Smesh-2.0) methodology of Shut-Down Dose Rate (SDDR) calculations

The MC model produced as result of T1 is supplied as input of T2, which integrates MC radiation transport and activation inventory calculation of the distributed decay gamma sources, and decay gamma transport, for SDDR calculations

1. MCNP neutron transport calculations to assess the spatial distribution of neutron spectra with mesh-tallies **– STEP 1**

FISPACT activation calculations using mesh-tallied neutron spectra and irradiation scenario:

- to quantify the generation of the radioactive nuclides in different materials;
- formation of the 3D decay gamma source covering a facility space of interest at required shutdown time

2. MCNP decay photon transport calculation to get the response from the source in the volume of interest and corresponding Shut-Down Dose Rates (SDDR) **– STEP 2**

T2 has to be used for the calculation of:

- **material activation**
- **transmutation**
- **detailed radioactive waste management**
- **Shut-Down Dose Rate**

[Ref. 3] M. Majerle et al., Verification and validation of the R2Smesh approach for the calculation of high resolution shutdown dose rate distributions, Fusion Eng. Des. 87 (2012) 443–447.

[Ref. 4] P. Pereslavtsev et al., Novel approach for efficient mesh based Monte Carlo shutdown dose rate calculations, Fus. Eng. Des. 88 (2013) 2719-2722

Example of neutronics analysis with two types of integration

T1 (CAD-to-MCNP conversion)
T2 (SDDR calculation with R2Smesh)

Example for SDDR analysis of the ITER Core Imaging X-Ray Spectrometer (CIXS) (Diagnostic system installed in ITER equatorial port)

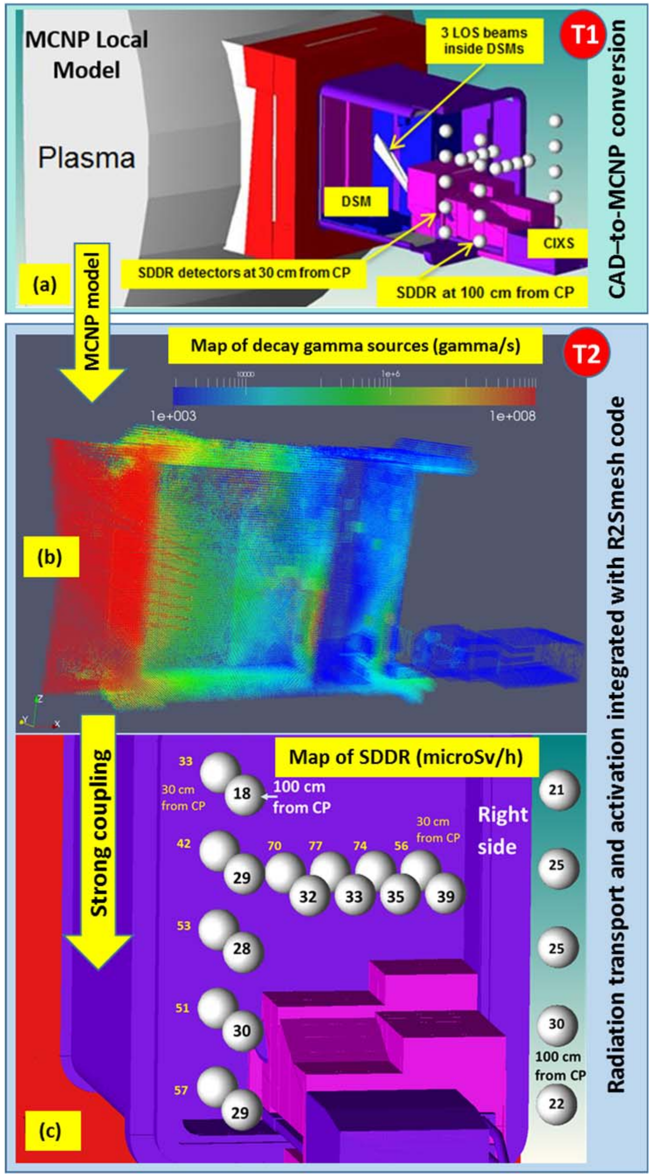
T1 is sufficient for the following calculations:

- neutron and photon fluxes
- nuclear heating (neutron and secondary photons)
- neutron damage (dpa)
- helium and hydrogen gas production

T2 should be used for the for the following tasks:

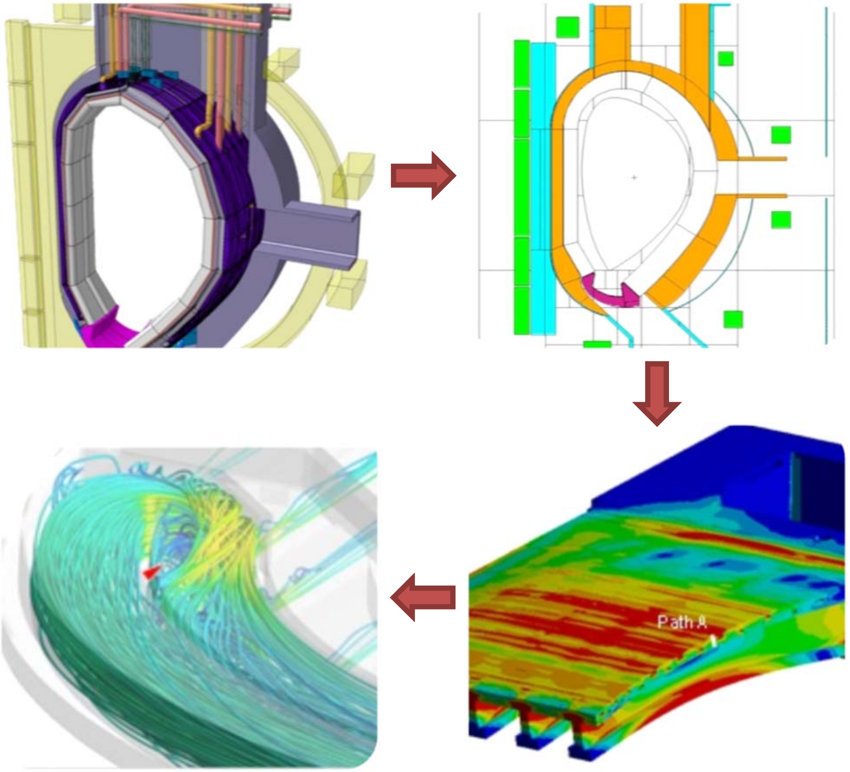
- material activation
- transmutation
- detailed radioactive waste management
- Shut-Down Dose Rate (SDDR) calculations

The detail T1 & T2 results of the ITER CIXS neutronics analysis:
[Ref. 5] A. Serikov et al., Neutronics analysis for the ITER core imaging X-ray spectrometer, Fusion Eng. Des. 109–111 (2016) 848–854



Need for integration: neutronics and heat loads & transfer

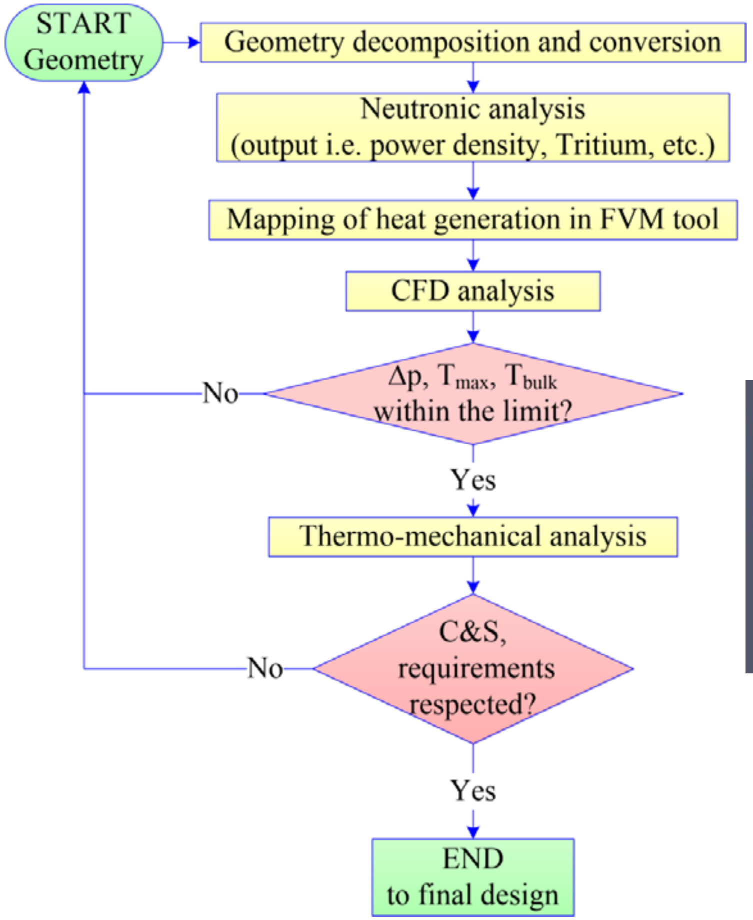
- Conventional coupling procedure used for the BB design:
  - Creation of generic CAD
  - Preparation of neutronic model (geometry details are not nodalised)
  - Neutronic output (i.e. radial power density) used for thermal-hydraulic and structural analysis **without feedback**



- Drawbacks:
  - Different geometry used by different models
  - The output of subsequent model does not feed back the previous one
  - Different teams with different background involved in the design
  - Time consuming and herald of errors.

MAIA = Multi-physics Approach for Integrated Analysis

Coupling procedure



START Geometry

Geometry decomposition and conversion

Neutronic analysis (output i.e. power density, Tritium, etc.)

Mapping of heat generation in FVM tool

CFD analysis

Δp, T_{max}, T_{bulk} within the limit?

No

Yes

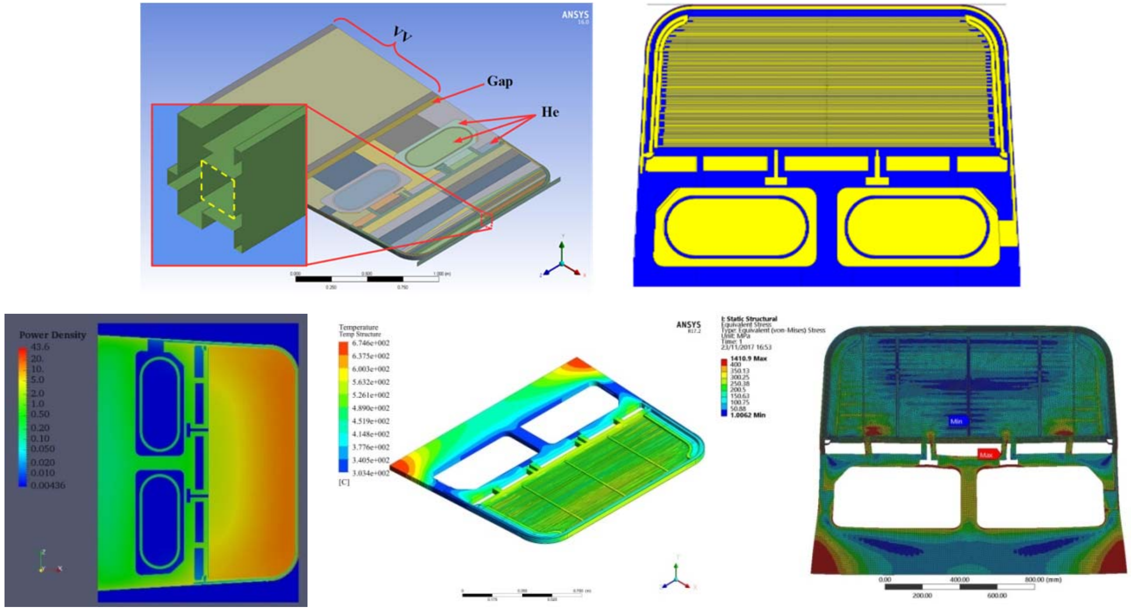
Thermo-mechanical analysis

C&S, requirements respected?

No

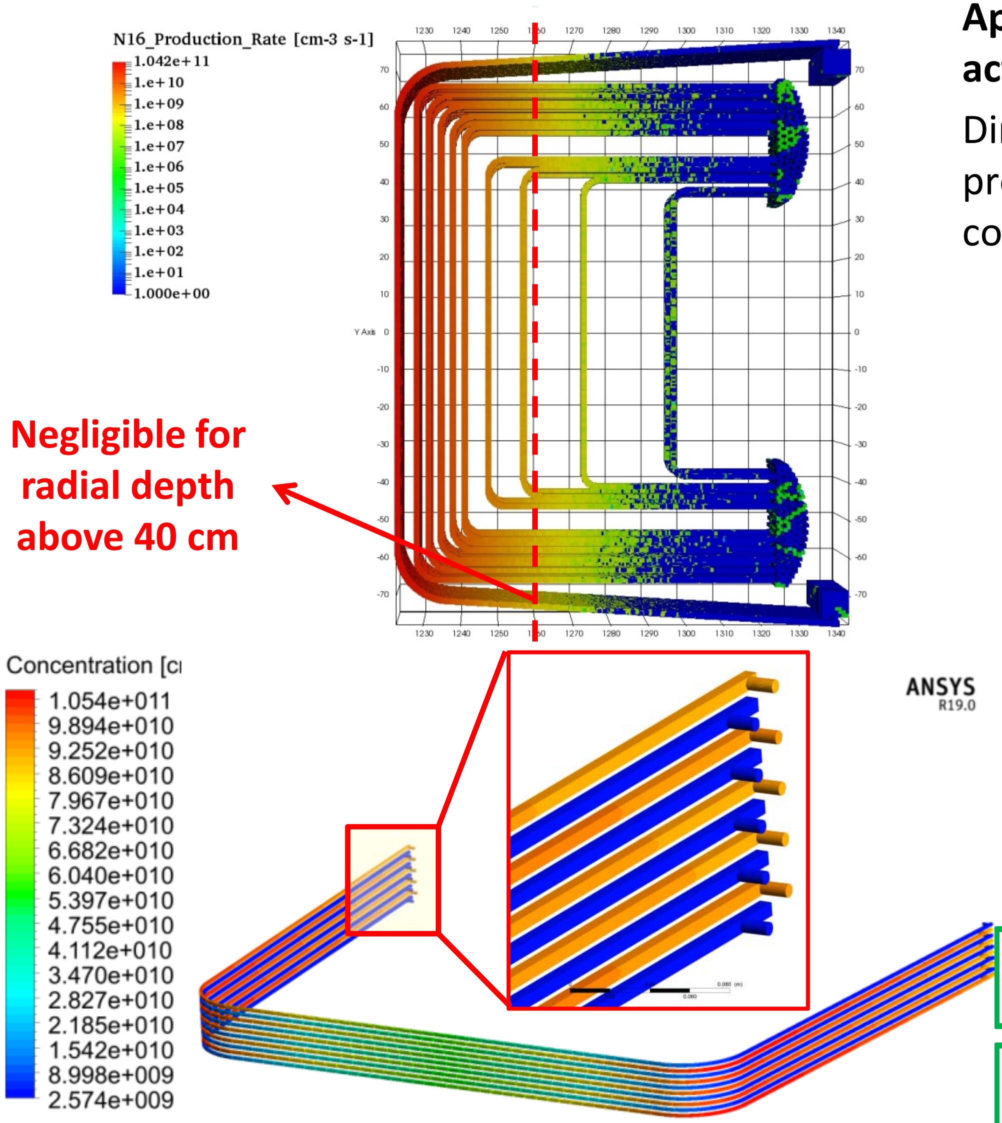
Yes

END to final design



MAIA is based on the coupling between ANSYS and MCNP

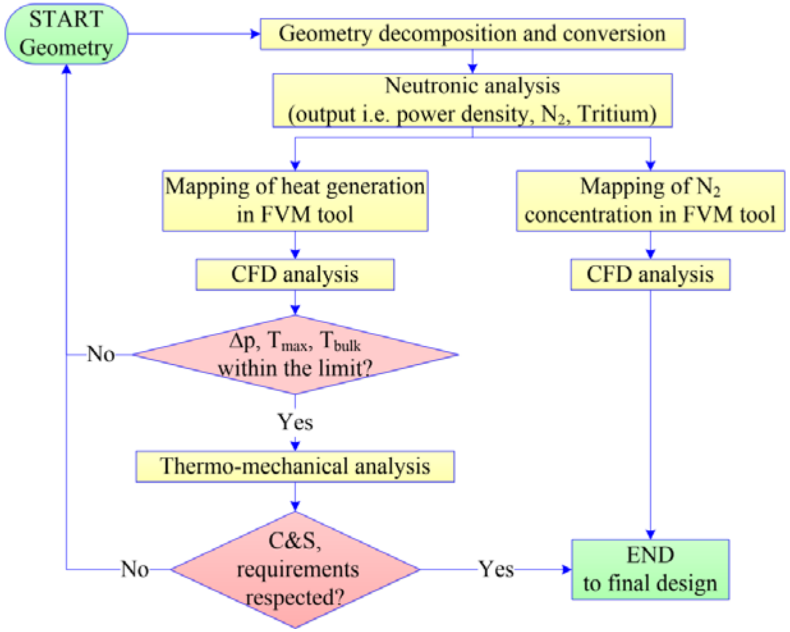
Enhancement of MAIA procedure



Negligible for radial depth above 40 cm

Application of MAIA procedure for water activation analysis.

Direct coupling of neutronic analysis (N isotopes production rate) and CFD calculation (3D N concentration distribution).



START Geometry

Geometry decomposition and conversion

Neutronic analysis (output i.e. power density, N_2, Tritium)

Mapping of heat generation in FVM tool

Mapping of N_2 concentration in FVM tool

CFD analysis

CFD analysis

Δp, T_{max}, T_{bulk} within the limit?

No

Yes

Thermo-mechanical analysis

C&S, requirements respected?

No

Yes

END to final design

P. Chiovaro et al., *Investigation of the DEMO WCLL Breeding Blanket Cooling Water Activation* (POSTER)

I. Moscato et al., *Assessment of the Dose Rates due to Water Activation on an Isolation Valve of the DEMO WCLL Breeding Blanket Primary Heat Transfer System* (POSTER)

Neutronics open issues are more experimental than computational

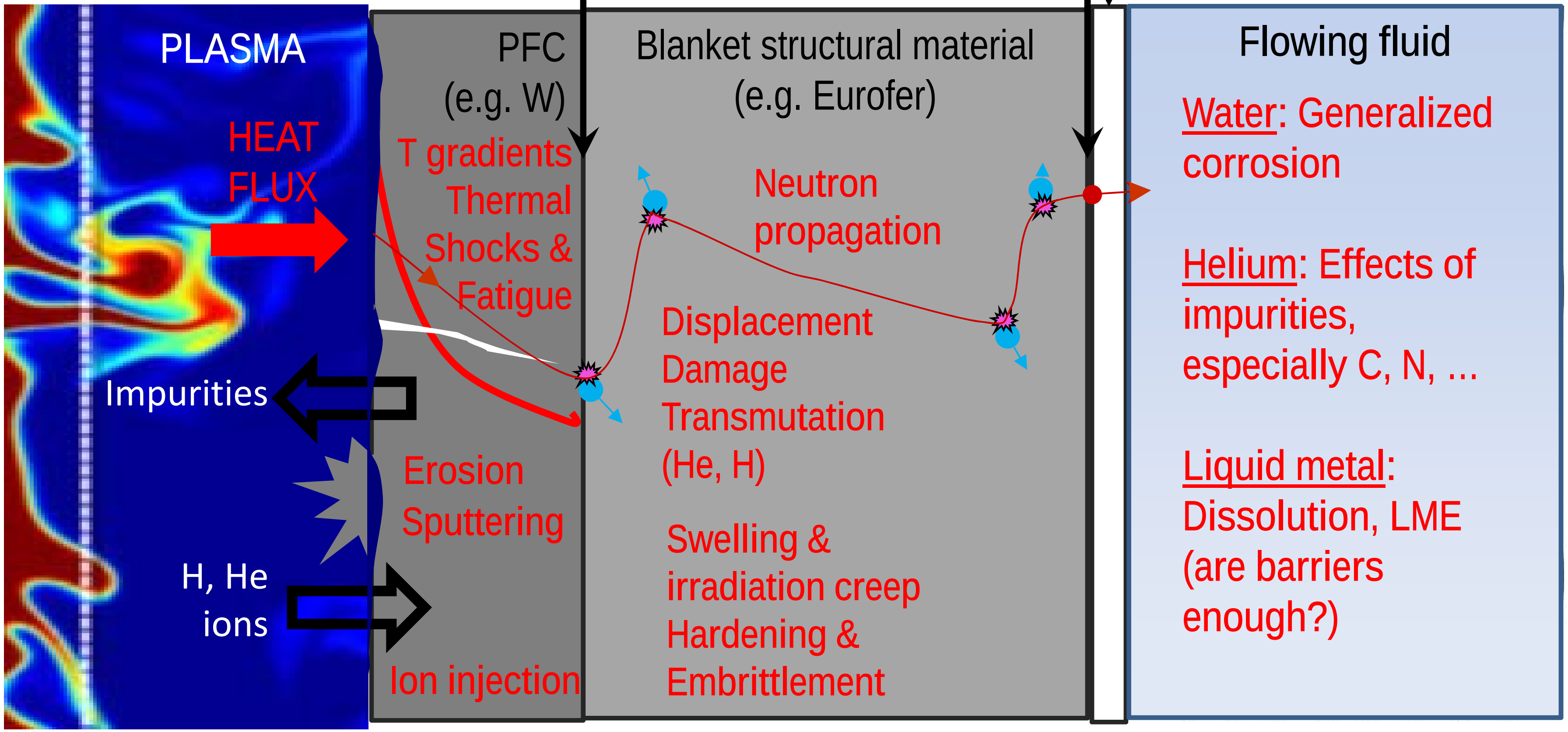
- **Volumetric neutron source** from D-T plasma. Right now we have 14 MeV neutrons from point D-T sources of neutron generators, accelerator-driven systems (ADS), Hohlraum capsule of National Ignition Facility (NIF), and so on. In all devices the source size is small.
- **Tritium breeding** for D-T fusion facilities beyond ITER. Requirement of tritium fueling system for **TBR is 1.05**. Engineering requirement for TBR is higher by 10%, it is **1.15** due to the need to compensate installation of non-breeding systems inside the ports with antennas of ICH, ECH systems, diagnostic systems, and so on.
- **T1 modelling challenges to reproduce CAD-based geometry** and all known physics phenomena are used in neutronics simulations in the form of nuclear cross-section data or models. The Monte Carlo (MC) method of radiation transport is the most suitable for complex, substantially heterogeneous geometry of fusion devices.
- **T2 activation-transport coupling schemes for SDDR.** The possibility to get the experimental results gained from facilities operated with D-T source is very dependent on maintenance access to particular areas, such as Inter-Space Structure (ISS) behind the port plugs. The safety of maintenance access is defined by the values of shut-down dose rates (SDDR) at those areas. Therefore, SDDR should be accurately estimated, taking account radiation transport and time-dependent activation phenomena.

Materials operating conditions

Thermal and damage gradients → internal stresses → cracking (integrity of interfaces/welds ?)

Interfaces / welds

T permeation and corrosion protection barrier (if relevant)



PLASMA

HEAT FLUX

Impurities

H, He ions

PFC (e.g. W)

T gradients Thermal Shocks & Fatigue

Erosion Sputtering

Ion injection

Blanket structural material (e.g. Eurofer)

Neutron propagation

Displacement Damage Transmutation (He, H)

Swelling & irradiation creep Hardening & Embrittlement

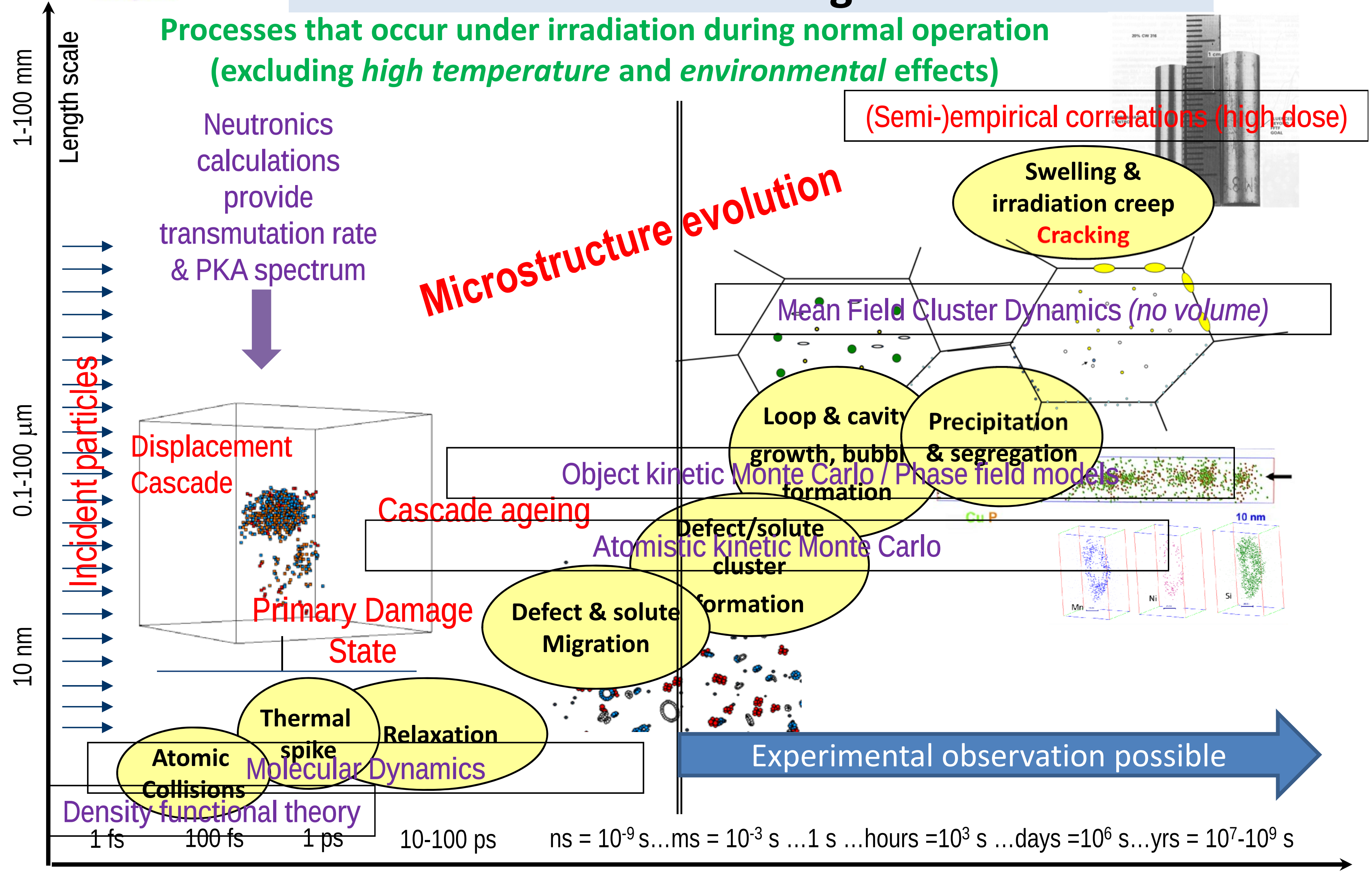
Flowing fluid

Water: Generalized corrosion

Helium: Effects of impurities, especially C, N, …

Liquid metal: Dissolution, LME (are barriers enough?)

Radiation effects - multiscale materials modelling



Processes that occur under irradiation during normal operation
(excluding *high temperature* and *environmental* effects)

(Semi-)empirical correlations (high dose)

Neutronics calculations provide transmutation rate & PKA spectrum

Microstructure evolution

Swelling & irradiation creep

Cracking

Mean Field Cluster Dynamics *(no volume)*

Loop & cavity growth, bubble formation

Precipitation & segregation

Object kinetic Monte Carlo / Phase field models

Displacement Cascade

Cascade ageing

Defect/solute cluster formation

Atomistic kinetic Monte Carlo

Primary Damage State

Defect & solute Migration

Incident particles

Thermal spike

Relaxation

Atomic Collisions

Molecular Dynamics

Density functional theory

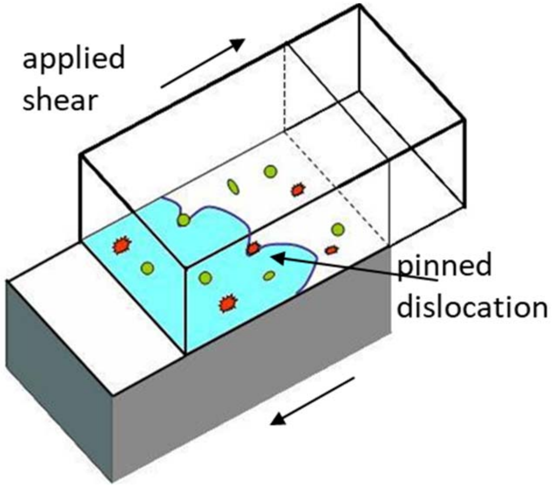
Experimental observation possible

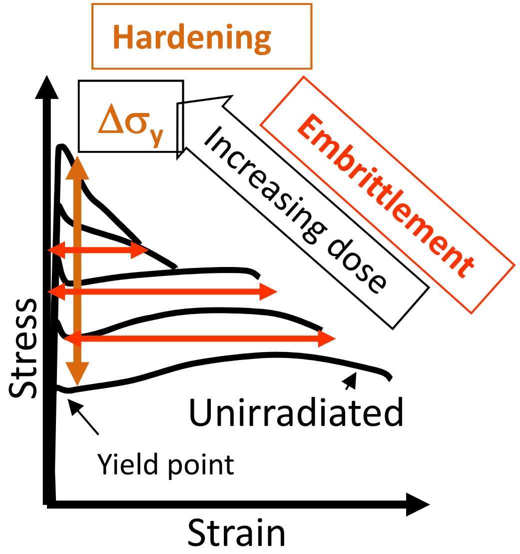
División de Materiales de Interés Energético

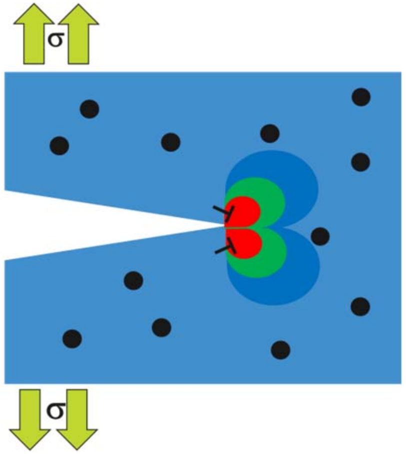
What happens if we test a material after irradiation? Change of mechanical properties

Timescale not really meaningful: strain at given strain-rate is the evolution variable

Radiation-induced hardening → embrittlement







Fracture models remain largely empirical

Dislocation-defect interaction / atomic-level

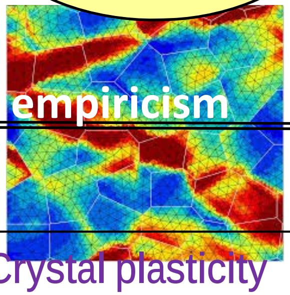
Dislocation-defect interaction / subgrain-level

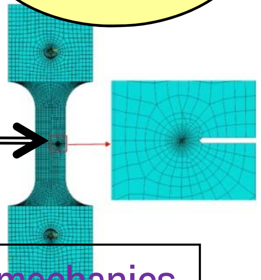
Dislo-dislo interaction / grain-level

Plastic Deformation / aggregate level

Plastic Deformation / specimen level

Fracture

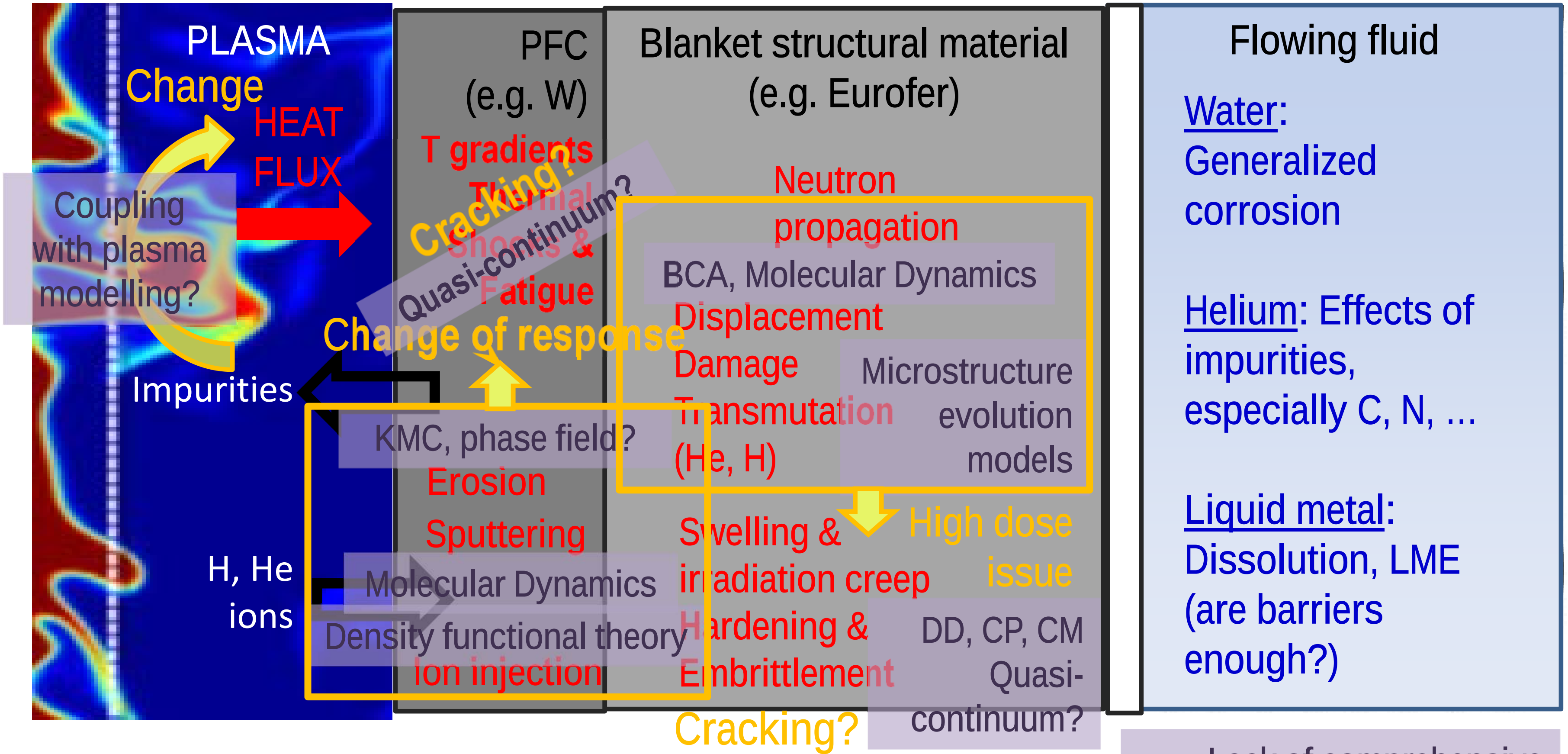




Increasing empiricism

Molecular dynamics	Dislocation dynamics	Crystal plasticity	Continuum mechanics	
10-100 nm	1-100 μm	1 – 100 mm	0.1 – 1 m	**Length scale**

Hypothetical couplings for a multiscale blanket materials modelling



Lack of physical mesoscale models describing internal stresses, crack initiation/propagation, ... He effects

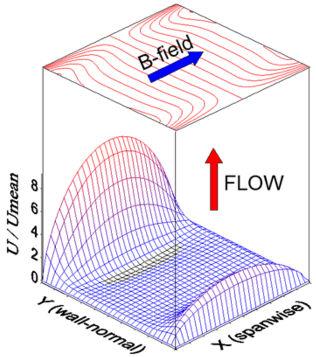
Lack of comprehensive mesoscale physical models for compatibility issues

Open issues and new trends

- Connect different scales:
  - Currently multiscale modelling = sequential use of single-scale tools with input from higher fidelity models
- Allow for effects of heterogeneity and chemical complexity:
  - Contradiction between averaging at higher scale and local phenomena triggering e.g. crack initiation
- Lack of full understanding of physical mechanisms:
  - True for most compatibility issues (e.g. IASCC, LME … effects of localisation? See above)
- Computational cost:
  - Limited representative volumes/timescales accessible to high fidelity models
- New trends:
  - Machine learning and data-driven modelling
- Possible strategy:
  - Filter information, remain with 1st order effects – physics cannot be forgotten
  - Take local information to higher scale (with the the help of machine learning?)
  - Deduce simple laws from complex problems (again with the help of machine learning?)

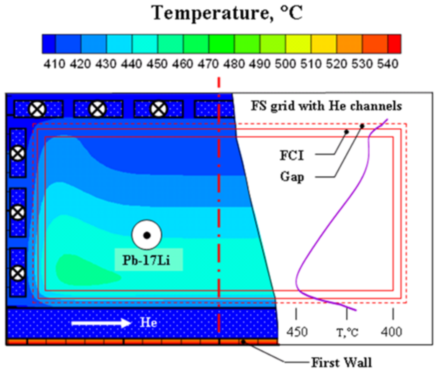
Liquid metal blanket design: MHD and Heat & Mass Transfer (transport processes) are primary drivers

- **MHD.** The motion of electrically conducting breeder/coolant in magnetic field induces electric currents, which interact with the magnetic field, resulting in strong Lorentz forces (4 to 5 orders of magnitude higher than hydrodynamic forces) that **modify the flow** in many ways.



Velocity and induced currents in MHD flow in a duct

- **Heat transfer.** The flowing LM and the surrounding structure absorb volumetric and surface heat resulting in high, strong-gradient temperature field in the liquid and the solid.

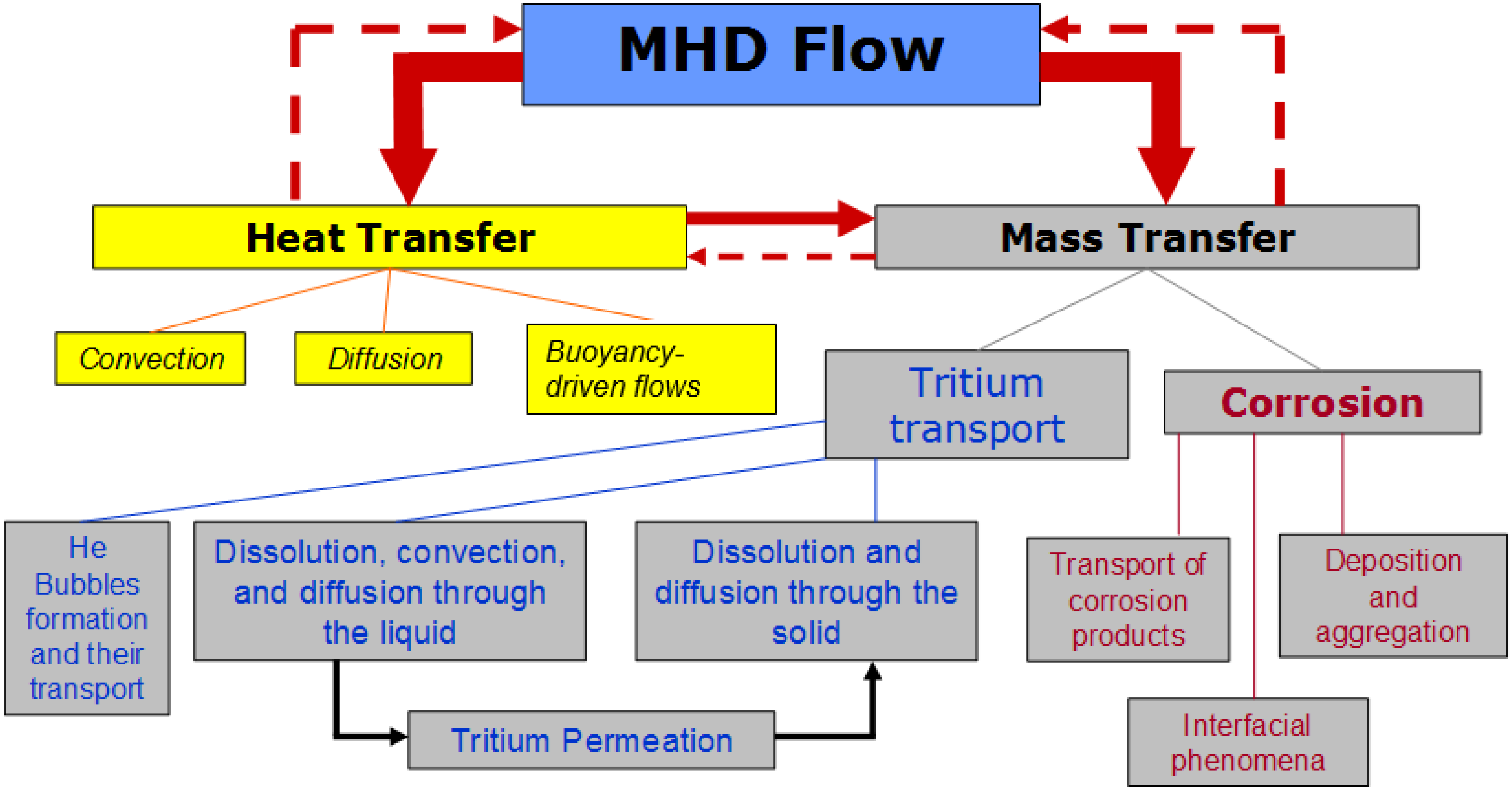


Temperature field in DCLL (ITER TBM)

- **Mass transfer. (1)** Li or PbLi are chemically aggressive, causing corrosion of structural and functional materials. **(2)** Once generated, Tritium is conveyed by the flowing LM and diffuses through the liquid and the solid.

Corrosion of RAFM in PbLi under B-field

In a LM blanket, MHD and Heat & Mass Transfer are non-linearly coupled leading to *multiple effects*



MHD Flow

Heat Transfer

Mass Transfer

Convection

Diffusion

Buoyancy-driven flows

Tritium transport

Corrosion

He Bubbles formation and their transport

Dissolution, convection, and diffusion through the liquid

Dissolution and diffusion through the solid

Tritium Permeation

Transport of corrosion products

Deposition and aggregation

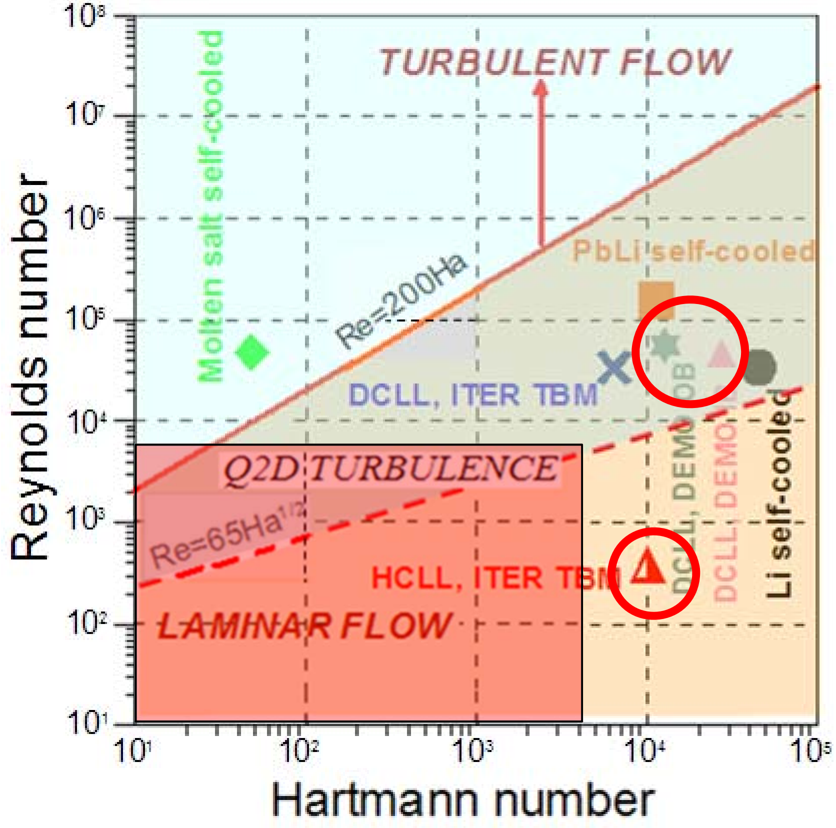
Interfacial phenomena

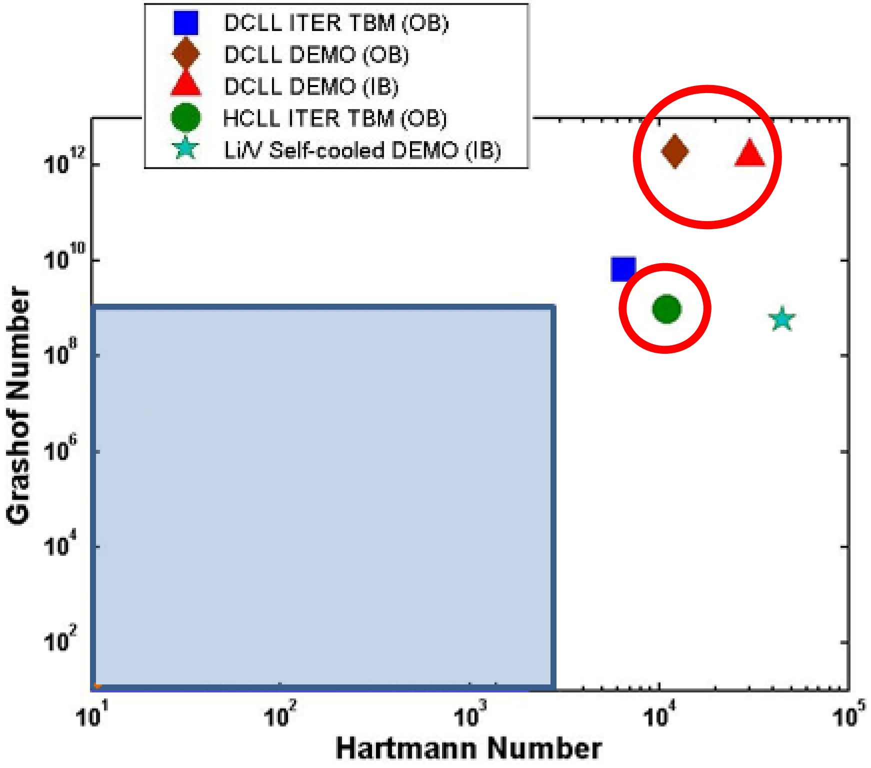
The simulation of these multiple effects in a blanket requires *INTEGRATED MODELING TOOLS*!

Which Computational Magneto-HydroDynamics tools are presently available?

I	Commercial multi-purpose CFD codes with buil-in/user-defined MHD module	• **FLUENT** – commercial multi-purpose CFD solver with a built-in MHD module • **CFX** – commercial multi-purpose CFD solver with a user-developed MHD module • **SC/TETRA** – commercial multi-purpose CFD solver with a built-in MHD module • **OpenFoam** – open-source multi-purpose CFD solver with a build-in electrodynamics module or user-developed MHD module
II	Massive non-commercial “home-made” solvers, especially developed for MHD applications	• **FLUIDYN** - CFD and multi-physics solver with build-in MHD capabilities by TRANSOFT International • **UCAS (China)** – “home-made” MHD solver with many computational capabilities • **HIMAG (USA)** - “home-made” MHD solver with many computational capabilities • **FEMPAR** (Spain, Badia et al.) – “home-made” multi-physics solver with MHD capabilities
III	Research codes limited to special type of flow and/or simple flow geometries	• **2D, Q2D and 3D research codes**, *e.g*. CoreFlow (L. Bühler, Germany), TRANSMAG (S. Smolentsev, US) • **DNS codes**, *e.g*. by Satake/Kunugi (Japan), Krasnov/Zikanov/Bueck (Germany)

Where are we now in CMHD?

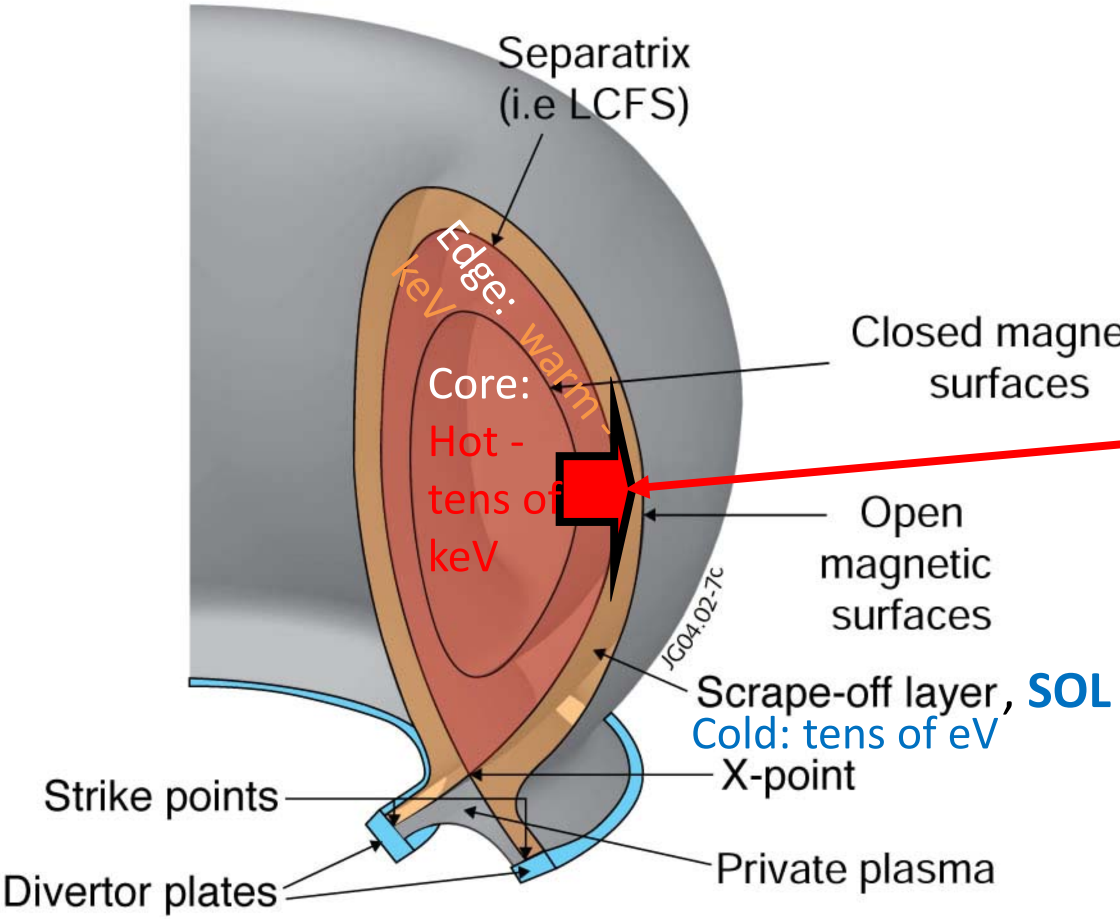




We are still pretty far from the target numbers

On the other side of the blanket/divertor: heat transfer from the plasma

Courtesy EFDA/JET



SOL:

- **Exhaust**
- **Fuelling**
- **Recycling**

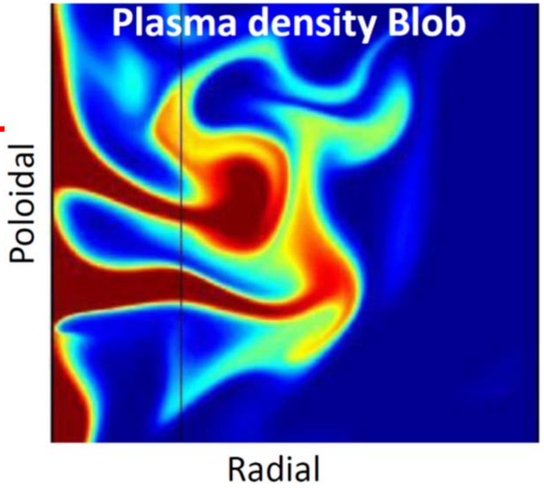
Main transport channel from confined plasma to SOL out-board-midplane

SOL transport is non-diffusive – Strongly intermittent

Cross field transport of particles and heat in magnetically confined hot plasmas is dominated by anomalous - turbulent - transport!

In the edge/SOL region the transport is strongly intermittent and characterized by:

- Large-amplitude, radially propagating magnetic field aligned filamentary structures – blobs – of elevated plasma pressure generated close to the last closed flux surface
- Resulting in localized power loads at plasma facing components
- Lasting influence on the chamber wall and other plasma facing components – particularly the divertor structures
- Strong demands on materials



Observed under a variety of conditions:

Zweben Phys. Fluids 28 974 (1985); Zweben *et al.* PPCF 49, S1 (2007); Garcia, Plasma Fusion Res. 4, 019 (2009); D'Ippolito *et al*. Phys Plasmas 18, 060501 (2011); Vianello et al. Nucl. Fus. 57 116014 (2017).

Modelling the SOL transport and plasma exhaust - wishlist

- **Multiscale** – from the parallel connection length (**tens of meters**) over the SOL plasma gap (**5-10 cm**), down to the power fall off length into the SOL and the wall sheath width (**mm**) and the ion Larmor radius (**sub mm**)
- **Multiphysics** – population of ”active” neutrals needs account for plasma / neutral interactions- elastic as well as in-elastic collisions – ionization, excitations etc.
- **Multi-ion species** –various hydrogen isotopes, helium, ions from gas puffs, impurities from sputtering of PFC.
- **Models** must encompass the edge and SOL region across Last Closed Flux Surface
- **No separation** between fluctuations and profiles - evolved on the same footing – fully non-linear description.
- **SOL -** open field lines end on material surfaces demanding sheath boundary conditions - may be implemented in a fluid description; but issues as detachment demand kinetic descriptions.

Edge/SOL dynamical codes

Several codes have been developed and applied during the last couple of decades

Typically based on four-field, drift-fluid models for vorticity, density, and electron and ion pressure with Braginskii closure for collisions [*e.g., Ricci, J. Plasma Phys. 81, (2015) 435810202*]

Examples:

SOLT [*Russell et al. Phys. Plasma 16 (2009) 122304*]

HESEL [*Nielsen et al. PPCF **59** (2017) 025012; Madsen et al. Phys. Plasmas **23** (2016) 032306*]

GBS [*Halpern et al. J. Comp. Phys. **315** (2016) 388*]

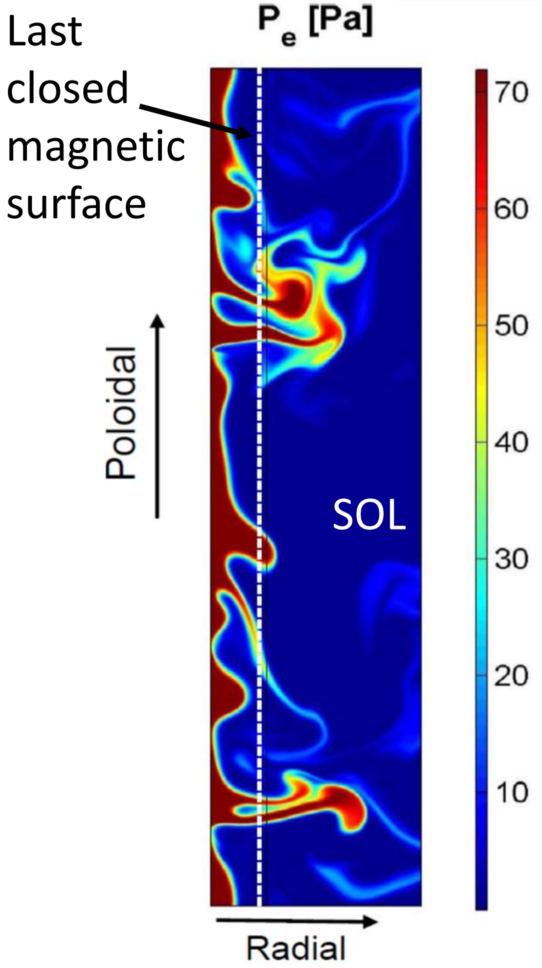
Hermes [*Dudson et al. PPCF **59** (2017) 054010*]

Tokam3X [*Tamain et al. PPCF **57** (2015) 0054014*]

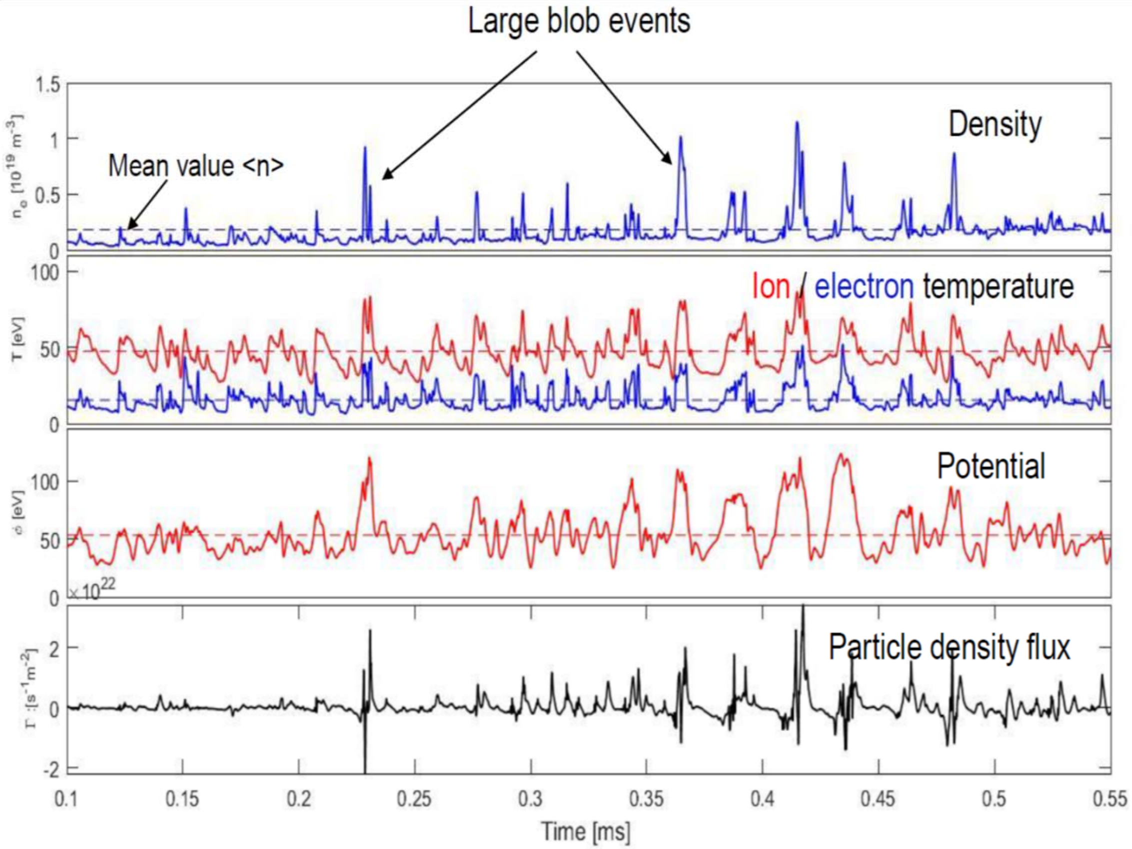
Examples from HESEL →

- ✓ **The codes predict plasma impact on material surfaces, including intermittent bursts – They provide:**
  - ✓ **heat source term for the design of the divertor and first wall**
  - ✓ **input for materials modelling**

Simulation of edge/SOL dynamics – blob evolution



Large blob events of significantly elevated electron pressure formed inside LCFS and propagating into the SOL.



Particle density, electron and ion temperature, plasma potential, and the particle density flux monitored at a "probe" in mid-SOL. Strongly intermittent ***fluctuations with peak values several times the mean value - make it difficult to predict the maximum heat flux***

Nielsen et al. Plasma Phys. Control. Fusion ***59*** *(2017) 025012*

Fusion reactor conceptual design

- During the early stages of reactor design:
  - Must **explore alternative designs**
  - Perform important **parameter trade-offs**
  - **Optimise** sub-system and reactor design and performance

- This is difficult if the **design time is of the order of months**…
  - Very **few** design **iterations**
  - Difficult to investigate alternatives

Need: Reactor design frameworks

- Replicate and **automate the reactor design process**
- **Accelerate** design point definition by orders of magnitude
- Enable **optimisation**

- Important because:
  - Can accelerate the design cycle and enable actual **optimisation** of reactor design and sub-systems
  - Can connect **various layers of knowledge and modelling** (e.g. from systems codes to neutronics codes) ensuring consistency between the different models we use to design reactors.

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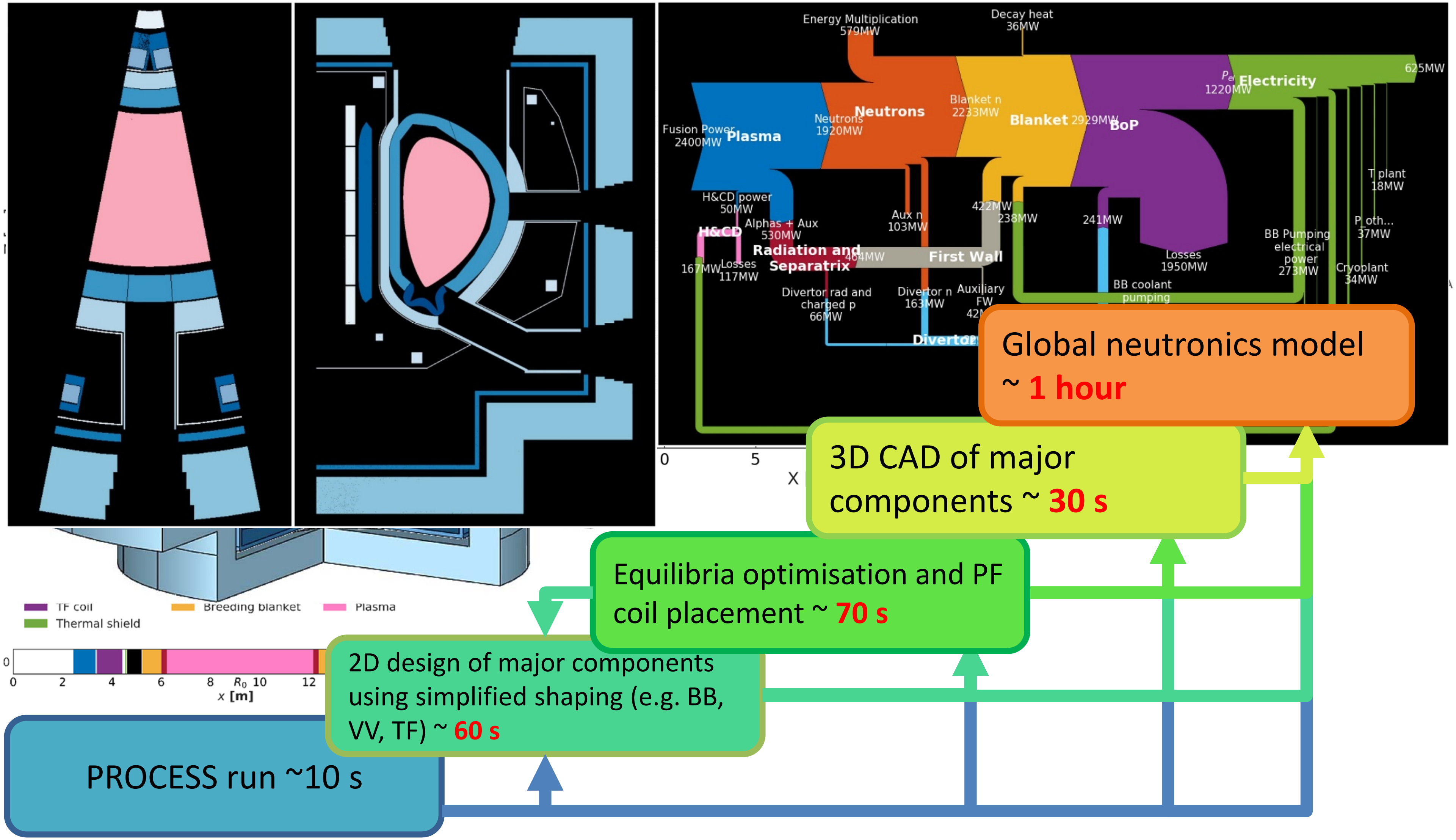
BLUEPRINT reactor design process (nutshell)



Global neutronics model ~ 1 hour

3D CAD of major components ~ 30 s

Equilibria optimisation and PF coil placement ~ 70 s

2D design of major components using simplified shaping (e.g. BB, VV, TF) ~ 60 s

PROCESS run ~10 s

BLUEPRINT: a novel approach to fusion reactor design

Are we ready to make an integrated computational tool to fully serve our needs?

- Despite significant progress in the development of computational tools in each particular area, integration into a single computational tool is premature as no component has reached the desired performance level
- Common requirements for each particular area:
    - *Multi-physics capability to cover a range of physical processes from single to multi-effect phenomena at different length scales*
    - *Efficiency and accuracy in reproducing the time-dependent behaviour with broad ranges of involved time scales*
    - *Ability to cover ranges up to high values of specific parameters (dimensionless numbers, neutron dose and dose-rate, stress and strain, temperature gradients …)*
    - *Ability to handle complex geometries*
    - *Sufficient computational speed*
    - *Complete verification and extensive validation*
- This should not stop from aiming towards a strong coupling of codes, even though the first attempts may need to be limited to simple coupling scenarios, or reduced computational models
- Integration strategies and attributes need to be evaluated in dedicated studies; at least in materials machine learning techniques may open new ways

On the role of integrated computer modelling in fusion technology

THANK YOU FOR YOUR ATTENTION

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