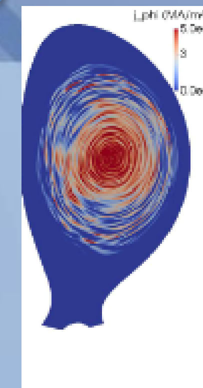
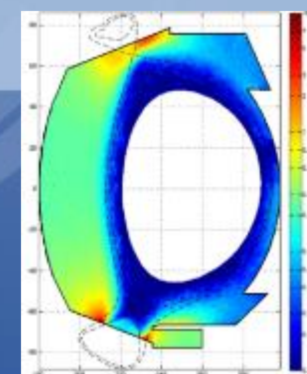
EUROfusion

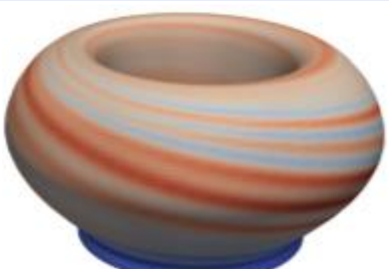
HPC-Marconi



EUROfusion-Theory and Advanced Simulation Coordination (E-TASC)



X. Litaudon on behalf of EUROfusion



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Acknowledgement to the E-TASC Scientific Board and TSVV Task Leaders

- E-TASC Scientific Board: B. Brams; R. Coelho; F. Jenko (chair); K. Nordlund, C. Roach, E. Serre; P. Strand, D. Tskhakaya, L. Villard; S. Wiesen, F. Zonca
- Theory, Simulation, Verification and Validation task leaders (2019-2020): D. Borodin, O. Embréus, T. Görler, J. L. Velasco, F. Schluck, P. Tamain
- EUROfusion Project Leaders members of E-TASC Scientific Board : S. Brezinsek; I. Calvo; F. Militello ; M. Coleman; J. Hillesheim; R. Kembleton, M. Wischmeier
- PMU: D. Borba, T. Donne, D. Kalupin, R. Kamendje, V. Naulin, M. Siccinio

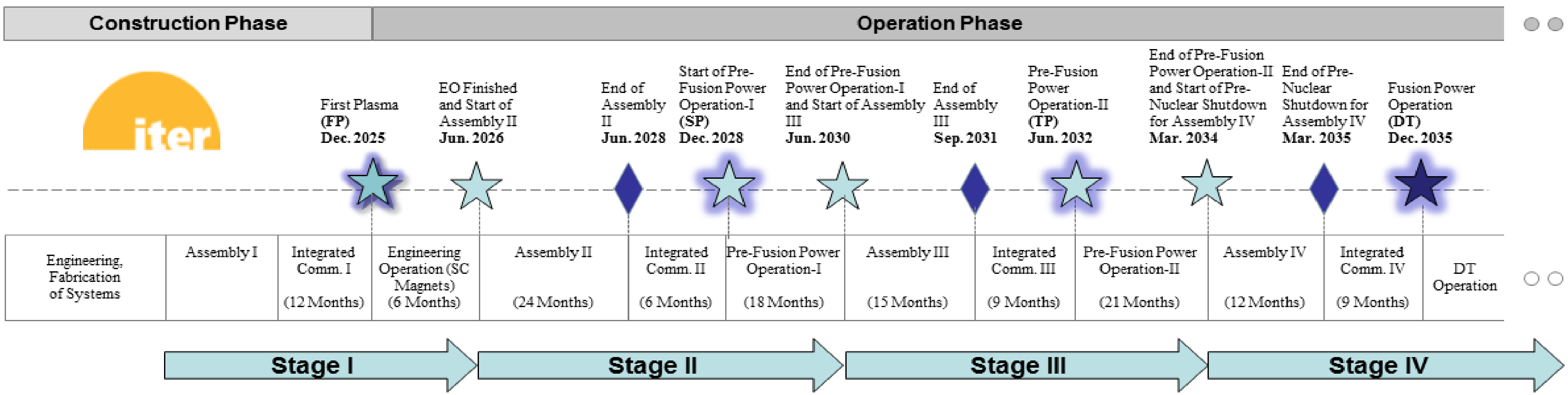
Background

- **Preparation of Horizon Europe**
  - EU to maintain an ambitious programme with a high level of leadership and coordination in the development of fusion energy
  - EU ready to play an important role in ITER scientific exploitation while finalising DEMO conceptual design
  - JET will be phased out while JT-60SA, ITER will start
- **Implementation of the Fusion Roadmap***
  - **"strong theory and modelling programme is essential because empirically-based predictions are uncertain in unexplored environments like ITER and particularly DEMO, and this will be a stronger focus than foreseen earlier"**

[*https://www.euro-fusion.org/eurofusion/roadmap/]

Major Changes during Horizon Europe

- **From ITER Construction to Operation**
  - Secure the success of future ITER operation
  - Prepare the ITER generation of scientists, engineers



[A. Loarte et al this conf.]

- **Prepare ITER operation and complete DEMO conceptual design**
- **with systematic simulation with different levels of sophistication**

Fusion theory-simulation in Nuclear Era

- **Nuclear facilities with safety and nuclear licensing issues**
- **Efficient, reliable, rapid design/prototyping for power plant**
- **Master operation with systematic modelling to save ~M€**
  - avoid ‘risky’ empirical approach
  - limited experimental time on ITER or test facilities
  - high operating cost (JET ~70M€/y , ITER ~300M€/y, DEMO …)
- **Master operation to ensure machine protection (~Billion€) and safety via control and validated algorithms schemes**
- **Theory/simulation (engineering/physics domain) has potential to accelerate the development of fusion energy**

We must prepare this transition with a coordinated, comprehensive theory/modelling/verification/validation programme by maximizing the benefit out of our facilities investment

Challenges to be addressed in Horizon Europe

- **Validated predictive capability of the L-H transition and pedestal physics in ITER and DEMO** (including ELMs, control and avoidance)
- **Validated predictive capability for heat exhaust in ITER and DEMO** (conventional/alternative divertor configurations)
- **Integrated scientific work on <u>plasma-wall interactions</u> in ITER & DEMO** (incl. HELIAS)
- **Integrated scientific work on <u>disruptions</u> in ITER & DEMO** (incl. their prediction, mitigation, and avoidance)
- **Integrated scientific work on <u>burning plasmas</u> in ITER & DEMO** (incl. HELIAS)

General principles of EUROfusion-Theory and Advanced Simulation Coordination (E-TASC)

- **Innovative theory and simulation research is performed when driven by the scientists and engineers themselves**
- **Nevertheless, the production of a new portfolio "EUROfusion standard software" requires a more directed approach**
- **To accommodate both, two inter-linked structures:**

  (1) Theory-Simulation-Verification-Validation (TSVV) Tasks

  (2) Advanced Computing Hubs which provide computer science, scientific computing, data management, code integration, and/or software engineering support for the TSVVs and the entire EUROfusion theory/simulation program → develop a new portfolio of EUROfusion standard software.

Healthy mix of coordinated de-centralized and centralized efforts in a virtuous cycle

E-TASC Scientific Board

TSVV Tasks

- M1, M8 Core-pedestal
- M2, M8 Pedestal-SOL, exhaust, PWI
- M3 Materials, neutronics
- M4-M7 Engineering

Advanced Computing Hubs

- Code integration, integrated modelling, and control (IMAS…)
- Code development and deployment on HPC
- HPC & mid-range facilities
- Data analysis (incl. AI) and management

EUROfusion "standard codes" for ITER operation and DEMO design

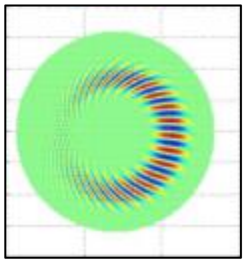
- Validated models for ITER & DEMO

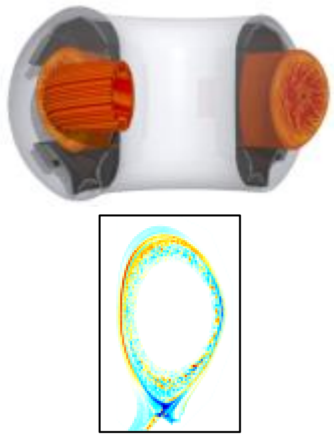
Advanced Computing Hubs

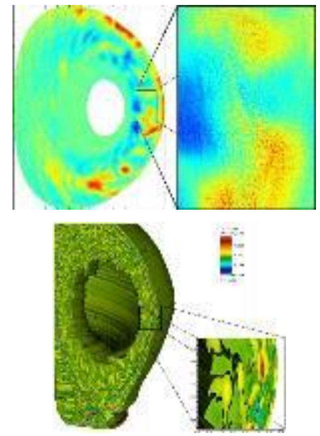
- **Call for proposals for hosting Advanced Computing Hubs**
  - Call issued **12/05/2020,** Deadline **08/01/2021**
- **Initiate up to five ACHs in 2021-2025 plus the JET data centre at DTU (Denmark)**
- **Cat. 1: High Performance Computing**
  - scalable algorithms, code parallelization and performance optimization, code refactoring, GPU-enabling, …
- **Cat. 2: Integrated Modelling and Control**
  - code adaptation to IMAS, IMAS framework development, code integration
- **Cat. 3: Data Management**
  - open access, data management, data analysis tools, aspects of AI and VVUQ
- **DTU (Denmark) has been already selected to host the JET data**
  - Agreement to be finalised end of 2020 for implementation in 2021

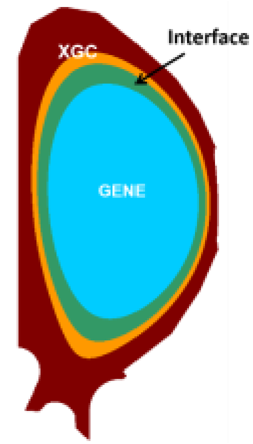
Towards virtual fusion systems

Increasing fidelity & modeling capability with increasing computing power









1990s
Gigaflops
Simplified physics in simplified geometry

Focus on core physics

2000s
Teraflops
Increasingly realistic physics in toroidal geometry

Also treating edge physics and electron scales

2010s
Petaflops
Multi-scale, multi-physics simulations

Core & edge are treated separately

2020s
Exaflops
Whole-device model of ITER, incl. turbulence, fast particles, MHD, heating, and plasma-wall interactions

Goals: Support **ITER operation** and **DEMO design**

[F. Jenko]

Theory-Simulation-Verification-Validation (TSVV) Tasks

- **Align with the Fusion Roadmap priorities and Missions**
- **Maximize the benefit out of our facilities investment**
- **Address high-priority issues (14 TSVV Tasks foreseen in FP9) for ITER operation and DEMO design:**
  - Advance understanding and predictive capabilities
- **Develop a high-quality suite of "EUROfusion standard" software**
  - To model data from EUROfusion facilities
  - To reliably extrapolate to future facilities: ITER / DEMO (including HELIAS)

Up 14 TSVV tasks to be initiated in Horizon Europe to address high-priority issues

Dep.	WP	#	Title
FSD	TE	1	Physics of the L-H Transition and Pedestals
FSD	TE	2	Physics Properties of Strongly Shaped Configurations
FSD	TE	3	Plasma Particle/Heat Exhaust: Fluid/Gyrofluid Edge Codes
FSD	TE	4	Plasma Particle/Heat Exhaust: Gyrokinetic/Kinetic Edge Codes
FSD	PWIE	5	Neutral Gas Dynamics in the Edge
FSD	PWIE	6	Impurity Sources, Transport, and Screening
FSD	PWIE	7	Plasma-Wall Interaction in DEMO
FSD	TE	8	Integrated Modelling of transient MHD Events
FSD	TE	9	Dynamics of Runaway Electrons in Disruptions and Start-Up
FSD	TE	10	Physics of Burning Plasmas + fast ions physics W7X
FSD	PrIO	11	Validated Frameworks for the Reliable Prediction of Plasma Performance and Operational Limits in Tokamaks
FSD	W7X	12	Stellarator Optimization
FSD	W7X	13	Stellarator Turbulence Simulation
FTD	DES	14	Multi-Fidelity Systems Code for DEMO

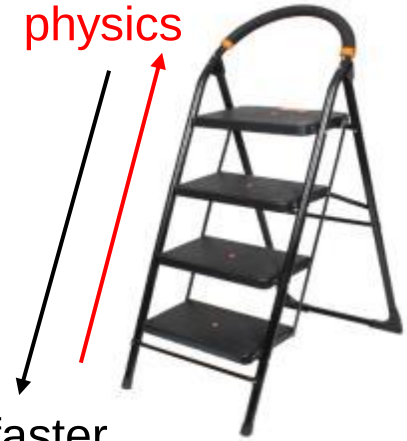
General remarks regarding all TSVV tasks

- **The goal is to provide validated predictive capabilities**
  - Turn existing research codes into professional and widely used tools
  - Develop new codes to fill some EU gaps (limited to a few select cases)
- **Multi-fidelity modelling** (first-principles-based models, corresponding reduced models, and novel multi-fidelity approaches) **as well as validation, verification, and uncertainty quantification (VVUQ)**
- **Validation and application involve a wide range of existing and future fusion devices**
- **Keep flexibility to launch new tasks or to close completed tasks**
- **Advanced Computing Hubs to provide support to entire EUROfusion simulation programme**

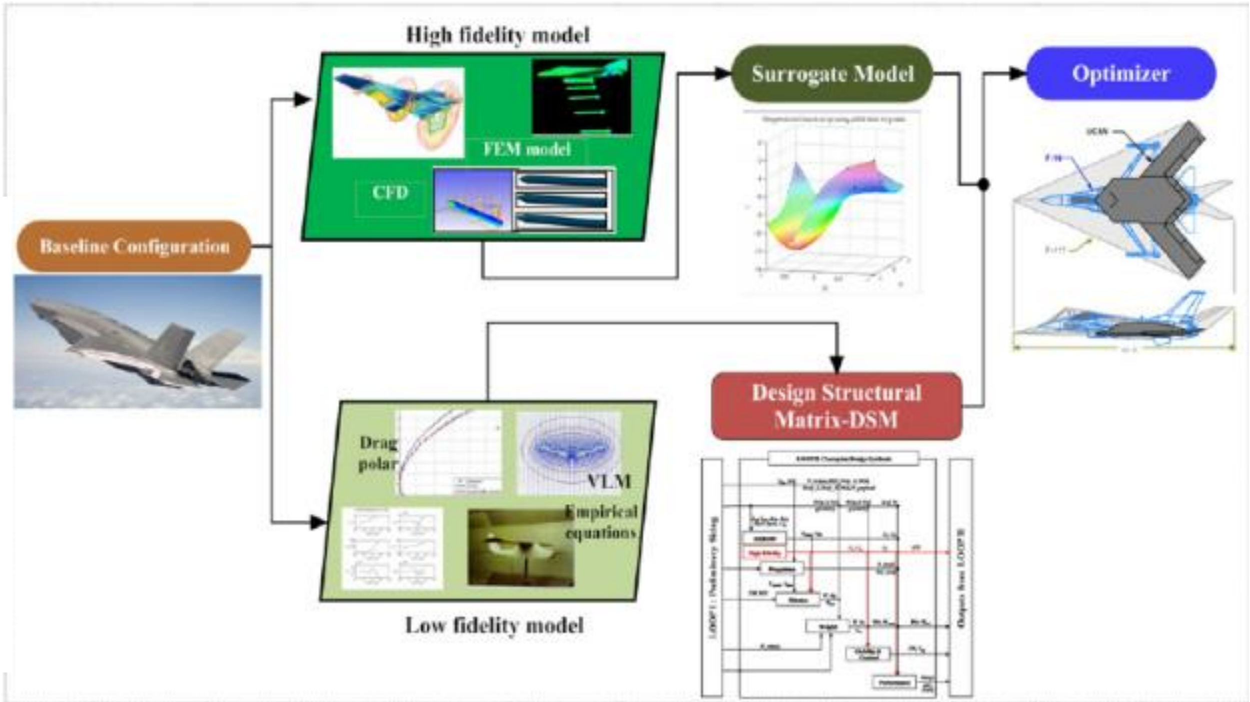
A multi-fidelity approach

An example:

more complete physics



faster simulations



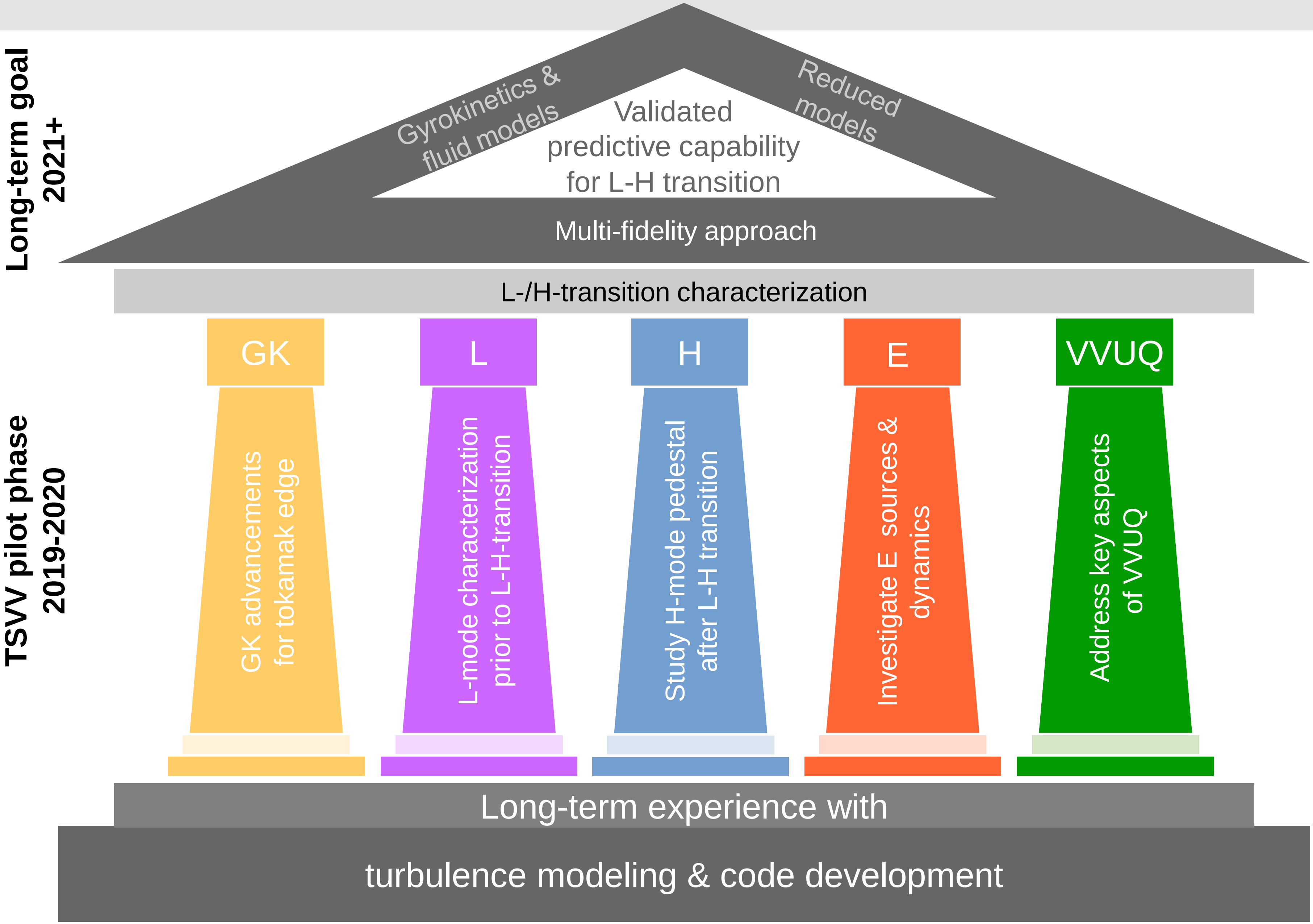
- High-fidelity models provide reliable **predictive capability**
- Lower-fidelity models foster **high-throughput computing**
- Both are needed – together and **simultaneously**

[F. Jenko]

5 Pilot tasks initiated early 2019 for two years

- **LH transition and pedestal physics**
  - Tobias Görler (MPG)
- **Electron runaway in tokamak disruptions in the presence of Massive Material Injection**
  - Ola Embréus (VR)
- **Fast code for the calculation of neoclassical toroidal viscosity in tokamaks (synergy Tokamak / Stellarator)**
  - José Luis Velasco (CIEMAT)
- **Neutral Gas Dynamics in the Edge**
  - Dmitriy Borodin/Friedrich Schluck (FZJ)
- **European edge and boundary code**
  - Patrick Tamain (CEA)

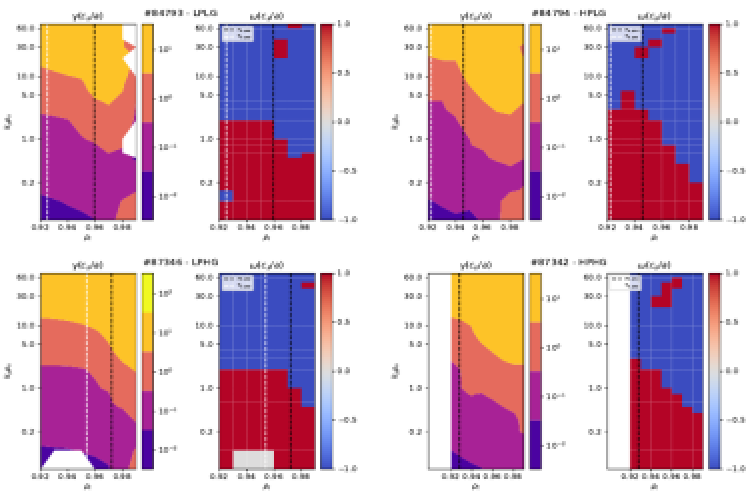
L-H transition and pedestal physics



Pedestal micro-instabilities: multi-codes/multi-machines characterization

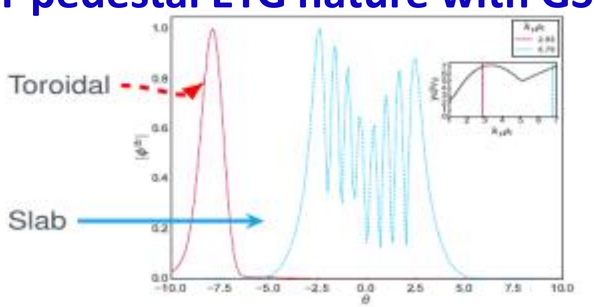
- **ETG modes dominant linear instability in the JET-ILW edge**
  - nonlinearly contribution to transport ?
- **Increased ITG instability in ASDEX-Upgraded argon seeded impurities**

GENE parameter scans JET-ILW



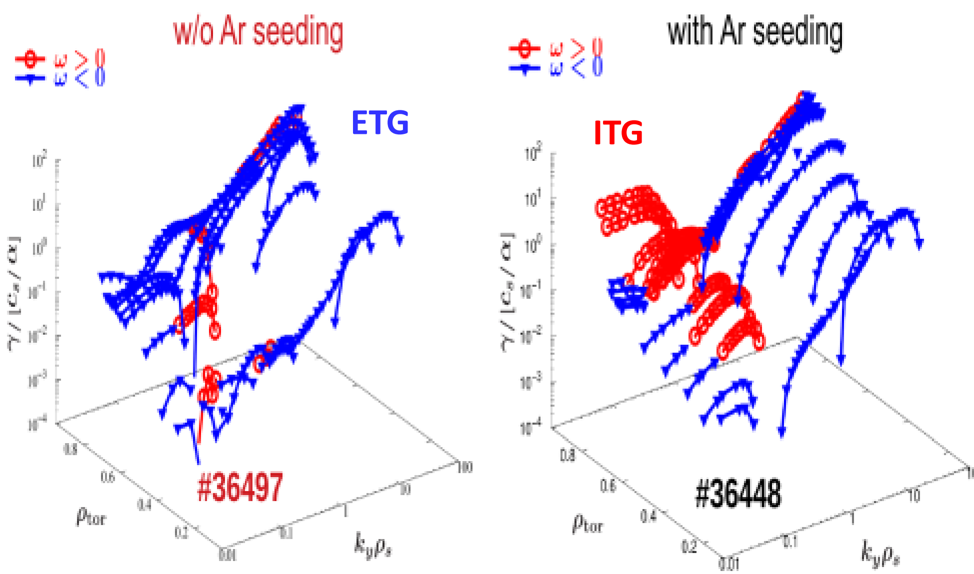
[Courtesy: Chapman]

JET pedestal ETG nature with GS2



[Courtesy: Parisi]

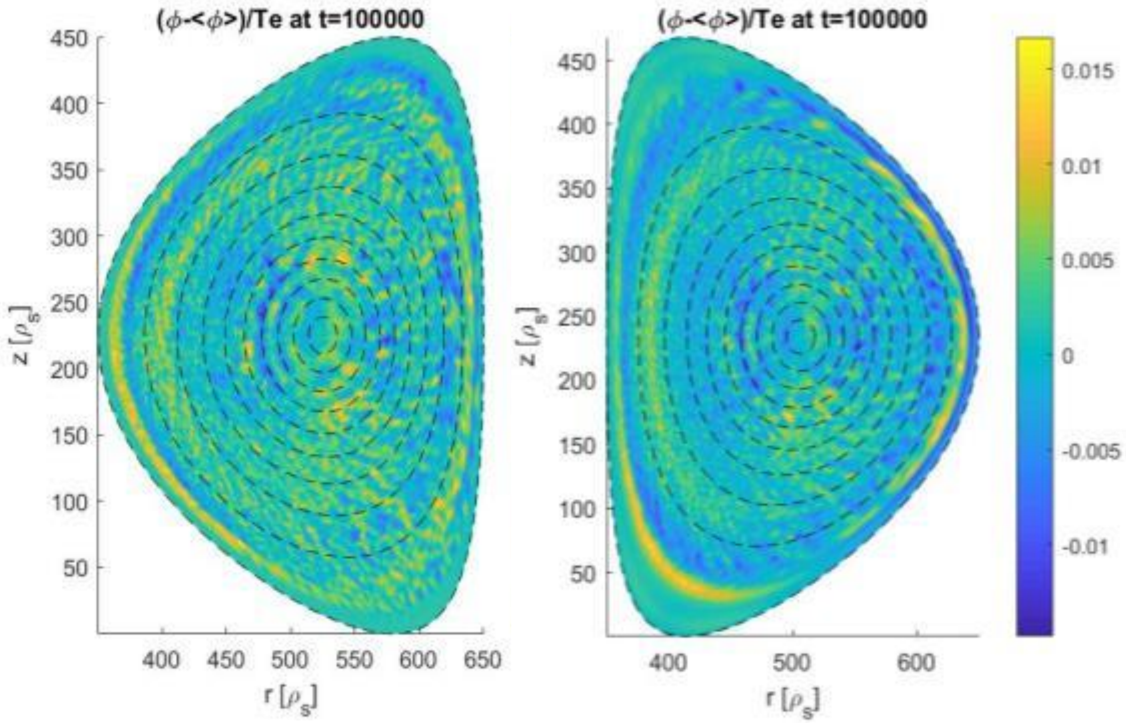
Micro-instabilities in AUG H-mode (GENE)



[Courtesy: Görler]

Gyrokinetic simulation of negative triangularity magnetic configurations on TCV

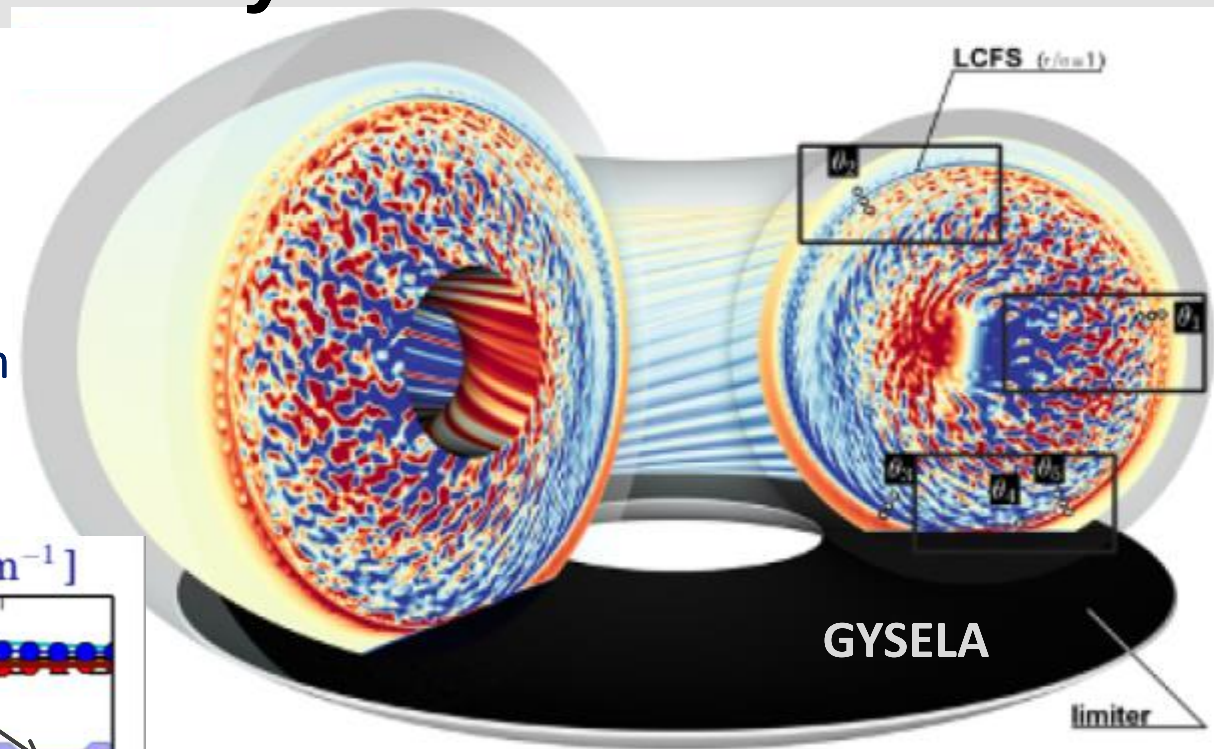
- **ORB5 is now able to simulate the plasma up to the very edge but assuming adiabatic electrons**
- **TCV discharges are Trapped Electron Mode dominated**
  - kinetic electrons need to be included to capture the transport reduction observed in negative triangularity configurations

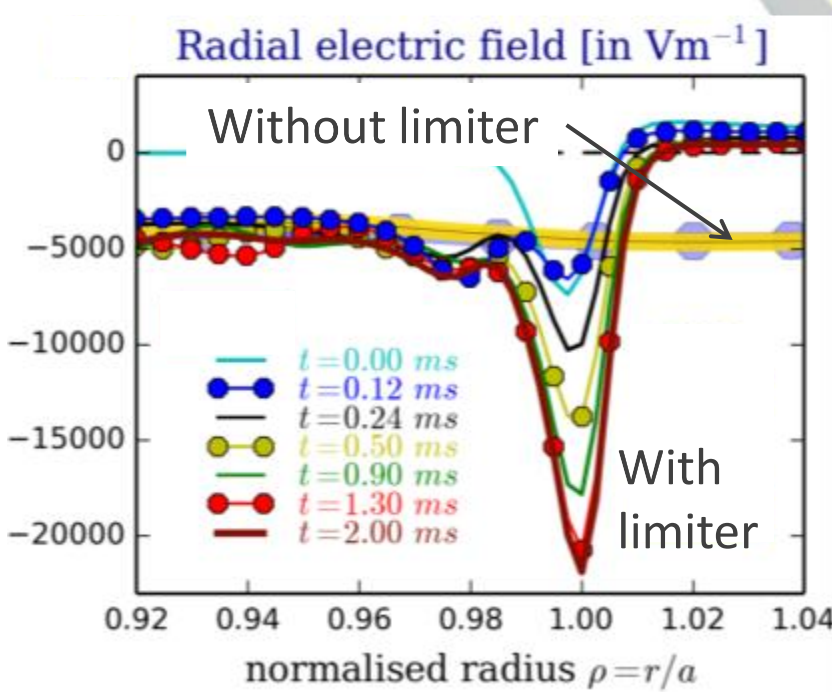


[Courtesy: Donnel]

Radial electric field well develops at separatrix with axi-symmetric limiter

- **Poloidally localized toroidal limiter**
  - Adiabatic electrons
  - Forced Bohm condition



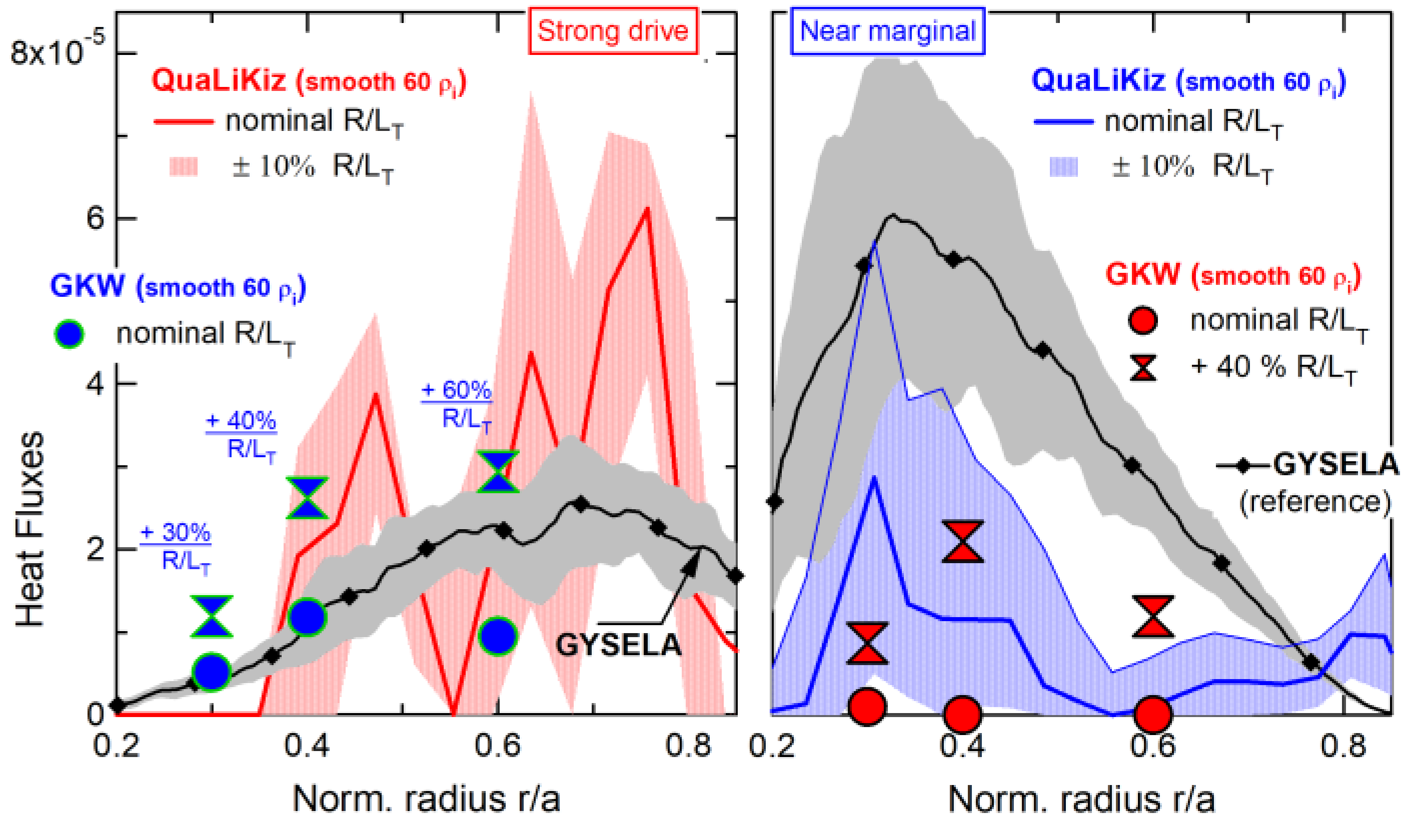


- **Radial electric field Well develops at separatrix**
  - mild steepening of pressure profile
- **Ongoing comparison with measurement**

[Courtesy: GYSELA team]

Towards reduced modeling: comparison of GYSELA, GKW & QuaLiKiz in two distincts turbulent ITG regimes

- **Good agreement in strong drive case with GKW & QuaLiKiz**
- **Important mismatch near marginality**

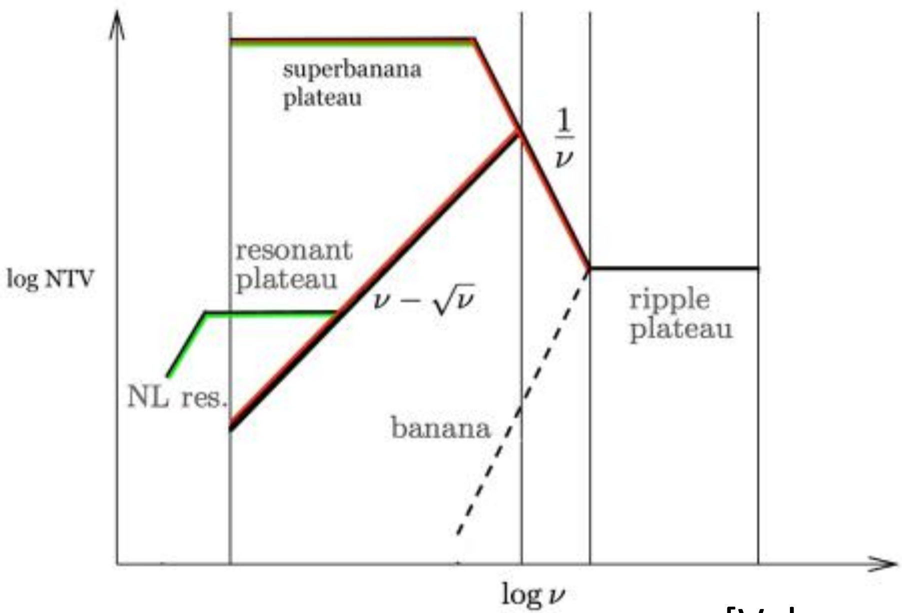


[Courtesy: GYSELA team]

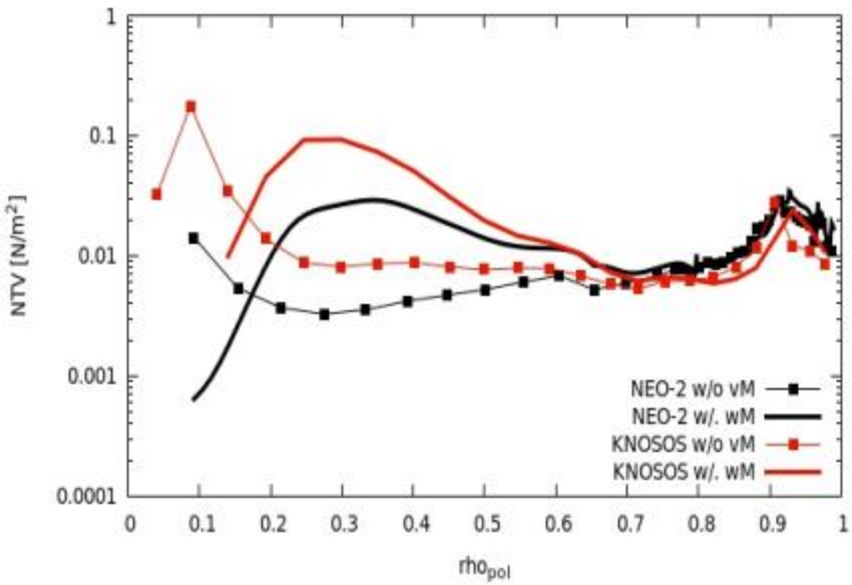
Calculation of neoclassical toroidal viscosity for tokamak and stellarator

- **Non-axial symmetry magnetic field can lead to neoclassical damping of the toroidal rotation**
  - Importance of proper estimate of neoclassical toroidal viscosity (NTV) in various collisionality regimes

KNOSOS, NEO-RT and NEO2 solve drift-kinetic equation for specific regimes



NTV simulations for ASDEX Upgrade



[Velasco et al., 4th Asia Pacific Conf. on Plasma Physics, 2020]

Disruptions and runaway electrons (RE)

- **Multi-scales disruption problem, involving:**
  - Non-linear resistive 3D MHD problem of the thermal quench
  - Generation, acceleration and radial transport of relativistic runaway electrons spanning energy scales across 6 decades
- **The combined problem remains an open challenge**
  - The project addresses each with a simplified account of the other
- **Objective is to develop:**

  (i) a comprehensive theoretical-numerical model framework to reliably predict RE dynamics in disruptions with non-equilibrium atomic physics for MST, JET and ITER,

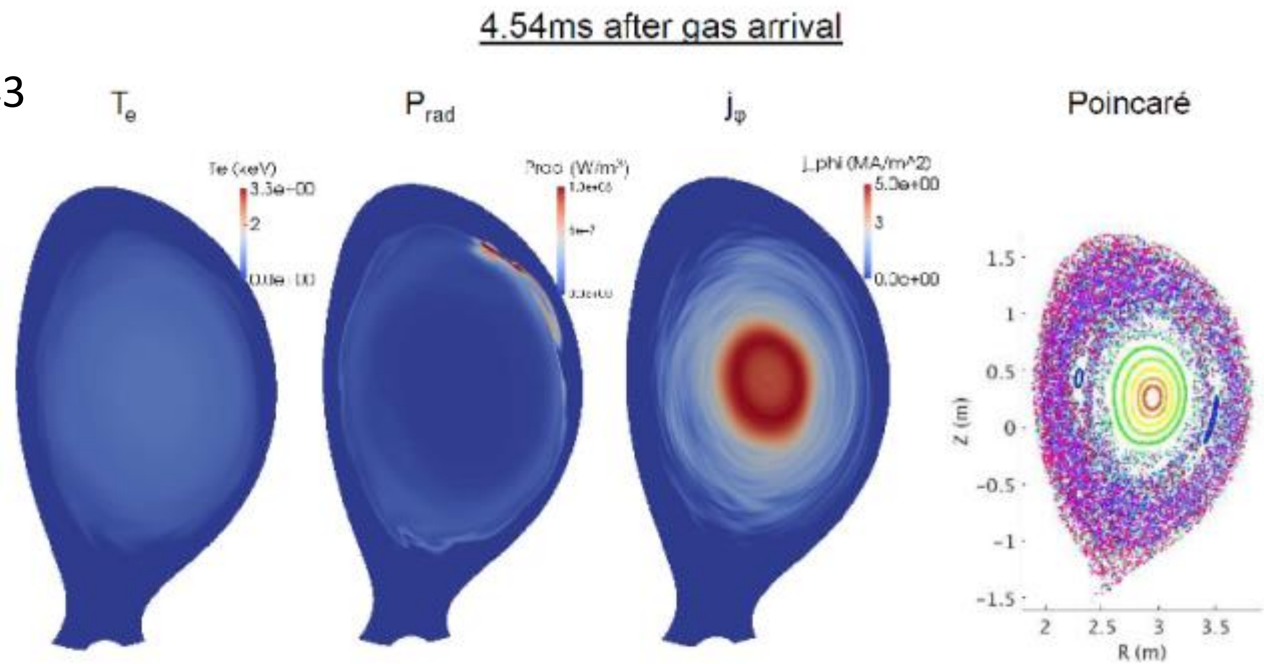
  (ii) a model of runaway mitigation by massive material injection and suggestions for improving RE mitigation,

  (iii) synthetic radiation diagnostic tools for validation.

Disruption: 3D non-linear MHD simulation

- **Thermal quench simulations with JOREK**
- **Material injection (argon) triggers kink-instability cascade**
  - Leading to magnetic field stochastication
- **Progress is being made in approaching realistic conductivity and viscosity to capture the measured current spike**

JET #85943



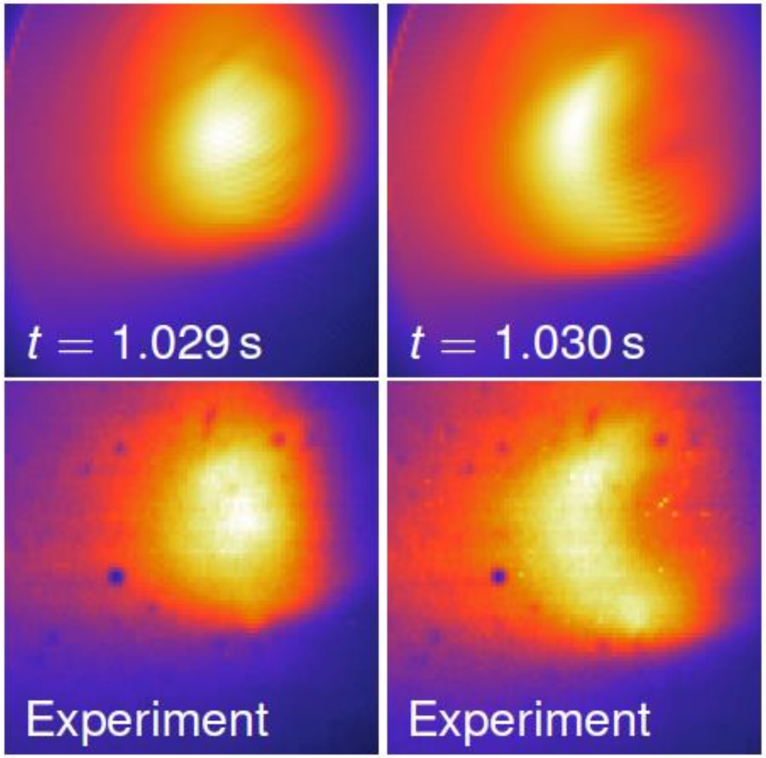
[Nardon 2019]

Runaways electron synchrotron radiation

- **Synchrotron emission provides information on RE dynamics**
- **Fokker-Planck forward modelling and RE distribution reconstruction inputs for synchrotron emission synthetic diagnostic**

Runaway radial distribution reconstruction [AUG #35628]

Synthetic (upper) and measured (lower) synchrotron images



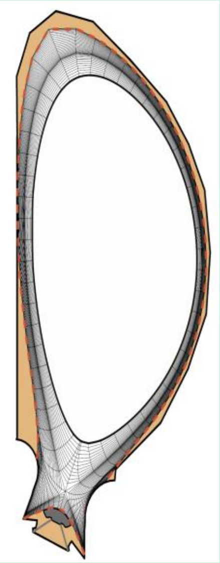
[M Hoppe et al NF (2020); M Hoppe et al. Accepted JPP (2020)]

Neutral Gas Dynamics: a hierarchy of neutral models

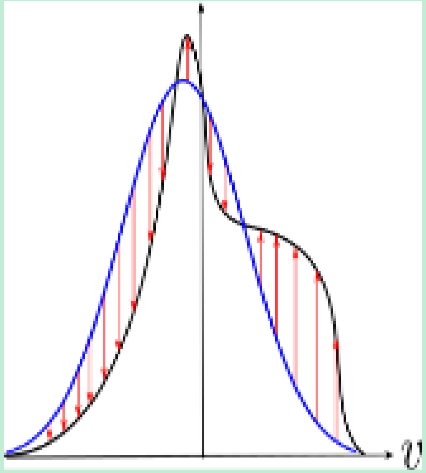
Advanced fluid neutral models

- Efficient (direct) coupling to plasma equations, no MC noise
- Basis for hybrid methods
- Good accuracy in highly collisional regimes

Hybrid fluid-kinetic models



- Decomposition in velocity space
- Can be made **equivalent** to kinetic model (!)



$$f_n(v) = f_{n,f}(v) + f_{n,k}(v)$$

Kinetic model

- Most complete physical description
- Flexibility w.r.t. geometry, collisional processes, sources, boundary conditions,…
- Very expensive in highly collisional regimes

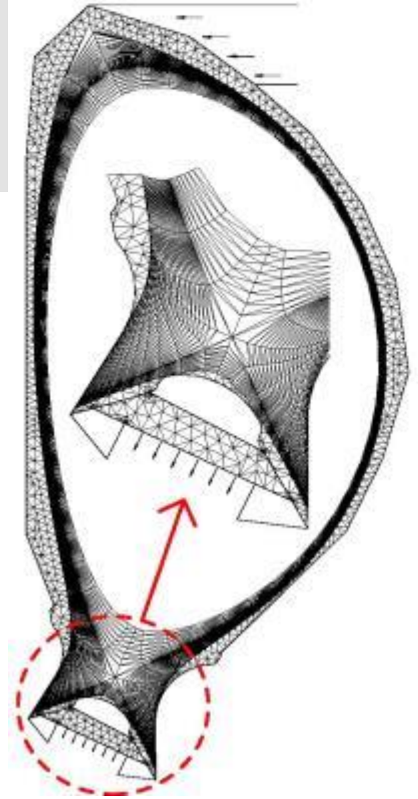
CPU × 1/10?

Model accuracy →

← Computational efficiency

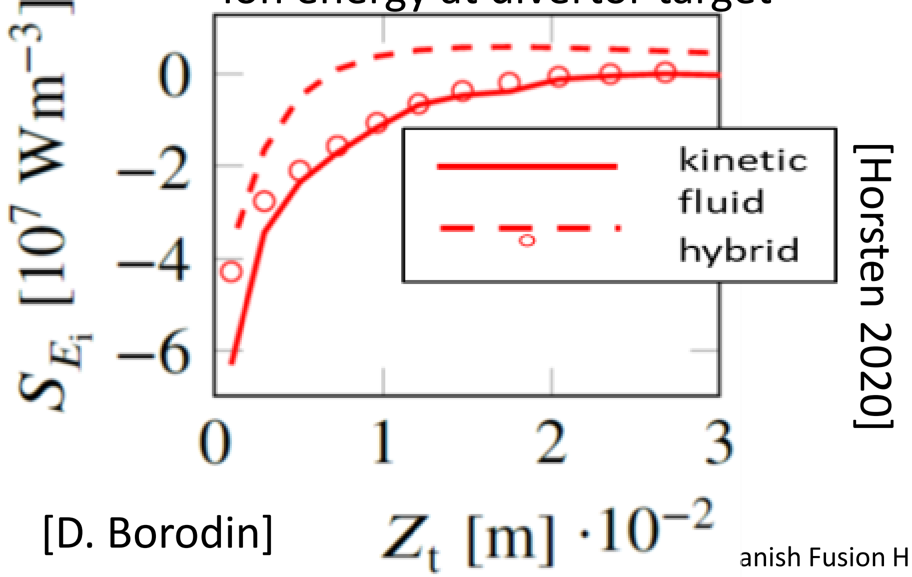
[D. Borodin]

Neutral Gas Dynamics in the Edge: Fluid-Kinetic Hybrid models



- **3D high fidelity simulation of neutral gas dynamics on ITER and DEMO computationally challenging**
- **Physics aspects**
  - Bring fluid and hybrid models for atoms as close as possible to full kinetic description: account for drifts, n-n collisions, and multi-species effects (H,D,T)
  - Investigate potential of fluid/hybrid models for molecules
  - Link to up-to-date databases for AMNS

Ion energy at divertor target

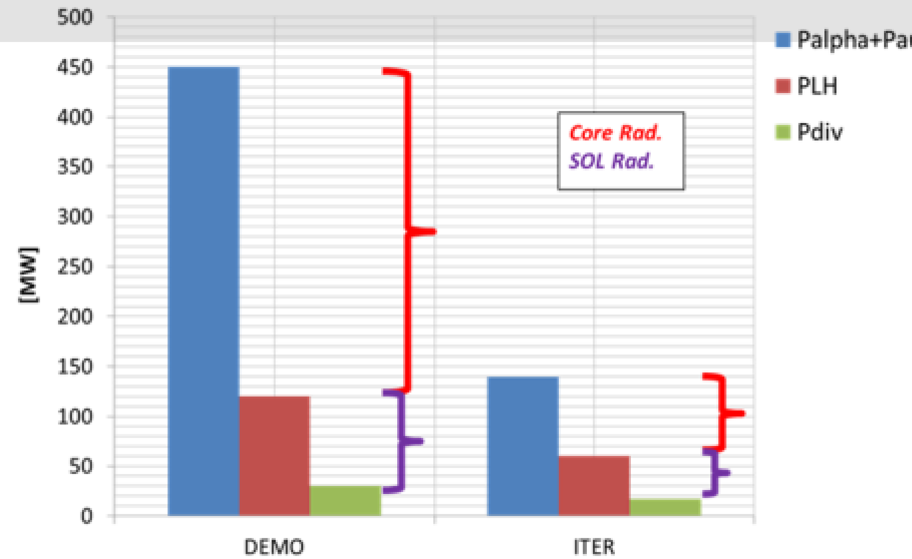


[D. Borodin]

- **Computation aspects**
  - Optimize hybrid algorithms to improve computational speed
  - Investigate potential of kinetic-diffusion Monte-Carlo schemes

European edge code for reactors?

- DEMO pushes the **power exhaust challenge** further
  - ✓ Strong constraints on operational space **margins**
  - ✓ **Uncertainties** on predictions
- **Limits of existing tools**
  - ✓ **Missing physics** hidden in free parameters (λ_q, S, flux limits…)
  - ✓ **Not enough computationally efficient** on modern HPC: MST case ~days, DEMO case ~months



	AUG	JET	ITER (Q=10)	DEMO
R_{geo} (m)	1.65	2.9	6.2	**8.8**
B_T (T)	2.5	2.6	5.3	**5.8**
I_P (MA)	1.2	2.5	15	**20.3**
n_{GW} (10^{20}m^{-3})	1.4	1.0	1.2	**0.8**
P_{heat} (MW)	26	25	150	**300**
$f_{rad,core}$	0.25	0.4	0.33	**0.5**
P_{sep} (MW)	20	16	100	**150**
P_{sep}/P_{L-H}	4.5	1.8	1.4	**1.1**
P_{sep}/R (MW/m)	12	5.2	17	**17**
$q_{\|} \propto$ **$P_{sep}B_0/R$ (MW·T/m)**	30	13	88	**99**
$c_z \propto$ **P_{sep}/B_p (MW/T)**	58	39	96	**138**

[P. Tamain]

[Reimerdes, 4th IAEA DEMO Prog. Workshop]

European edge code development: high level objectives

- Ensure predictive capability for heat and particle exhaust up to reactor relevant conditions
- Design and physics studies (not engineering code) in a multi-fidelity approach
  - Hierarchy of models => user can compromise fidelity vs computing time
  - Designed to run on exa-scale architectures for large cases
  - Aim at ~month duration simulations for most advanced models

Requires simultaneous progress on the

physics, algorithmic and HPC optimization sides

[P. Tamain]

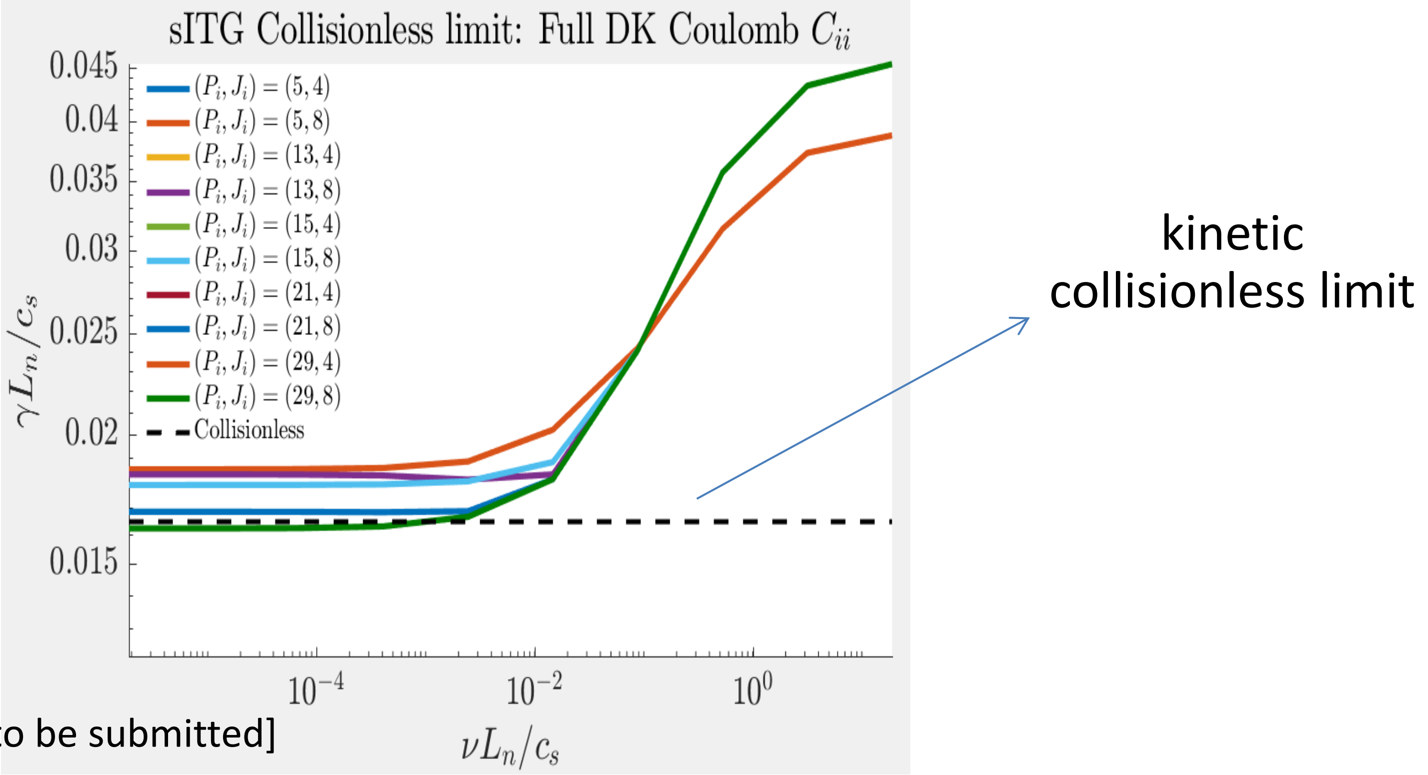
Key challenges

- **Develop plasma model compatible with reactor conditions**
  - **4 decades collisionality range** (divertor to pedestal) beyond domain of applicability of standard fluid models [c.f. next slide]
- **Integrate reactor relevant physics**
  - additional physics in turbulence models for consistent environment (neutrals, impurities…)
- **Optimize codes for HPC**
  - In pilot phase, focus on optimization of common bottleneck of existing codes: elliptic solvers for plasma potentials
- **Optimise algorithms and computational needs**
  - Advanced parallel discretization methods based on Flux Coordinate Independent approach [Hariri CPC 184 (2013), Stegmeir CPC 198 (2016)]
    - reduction of computational needs (mesh resolution and time step)
  - Pilot Phase: Hybrid Discontinuous Galerkin approach under development

Recent progress on plasma model in DEMO conditions at low collisionality

ITG linear growth rate as versus collisionality

- different truncatures level in the gyrofluid moment hierarchy with full nonlinear gyrokinetic Coulomb collision.



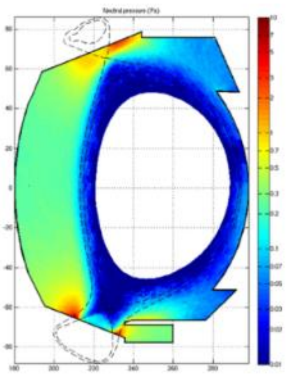
[Frei, Jorge & Ricci, JPP, to be submitted]

- **If enough moments in the N-moments gyrofluid model: collisionless kinetic regime is recovered !**

HPC efficiency is critical

Two orders of magnitude larger than current record

Computational Fluid Dynamics (CFD) Simulation



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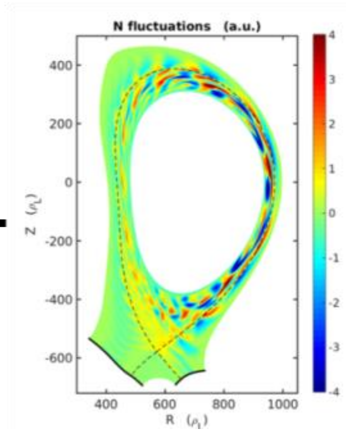

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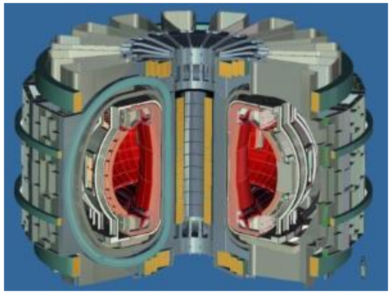

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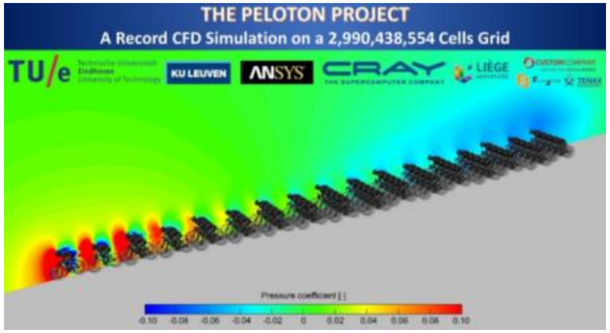

Neutrals, impurities, realistic geometry

3D turbulence

DEMO:

$> 2\ Billion$ degree of freedom (dof) per poloidal plane

$> 200\ Billion\ \ dof$ for 3D domain

- **<u>Rough</u> estimate of computing power needs for DEMO application:**

$R \approx 10m,\ a \approx 3m,\ \Delta r \approx 10cm$

$\rho_L \approx 0.05 - 0.7\ mm \qquad [3 \times (> 20)\ ionized\ species] > 60\ fields$

[P. Tamain]

Conclusion

- **Theory & advanced simulation** – which are "essential because empirically based predictions are uncertain in unexplored environments like ITER and particularly DEMO" – **has found a home within EUROfusion: E-TASC**
- **Theory & advanced simulation** can save many M€/y in operational cost, help to ensure machine protection, and has the potential to accelerate the development of fusion energy
- Via a synergy between **Theory-Simulation-Verification-Validation (TSVV) Tasks** and **Advanced Computing Hubs**, **E-TASC** will develop validated predictive capabilities for key challenges in fusion research for ITER and DEMO
- **Progress will rely and should adapt to the evolution of computing resources for large scale simulation and integrated modeling**

Thank you for your attention on behalf of the EUROfusion contributors

ÖAW Österreichische Akademie der Wissenschaften
Austrian Academy of Sciences
AUSTRIA

Ecole Royale Militaire Laboratory for Plasma Physics
BELGIUM

Bulgarian Academy of Sciences
BULGARIA

Ruđer Bošković Institute
CROATIA

University of Cyprus
CYPRUS

IPP ASCR
Institute of Plasma Physics Academy of Sciences of the Czech Republic
CZECH REPUBLIC

DTU
Technical University of Denmark
DENMARK

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University of Tartu
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Max-Planck-Institut für Plasmaphysik
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National Center for Scientific Research "Demokritos"
GREECE

wigner
Wigner Research Centre for Physics
HUNGARY

DCU
Dublin City University
IRELAND

ENEA
Agenzia nazionale per le nuove tecnologie, l'energia e lo sviluppo economico sostenibile
ITALY

Latvijas Universitāte
University of Latvia
LATVIA

LEI
Lithuanian Energy Institute
LITHUANIA

IFPiLM
Institute of Plasma Physics and Laser Microfusion
POLAND

Instituto Superior Técnico
PORTUGAL

ifa
Institute for Atomic Physics
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EPFL
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École polytechnique fédérale de Lausanne
SWITZERLAND

FOM
Foundation for Fundamental Research on Matter
THE NETHERLANDS

CCFE Culham Centre for Fusion Energy
UNITED KINGDOM

KIPT
UKRAINE

Back-up

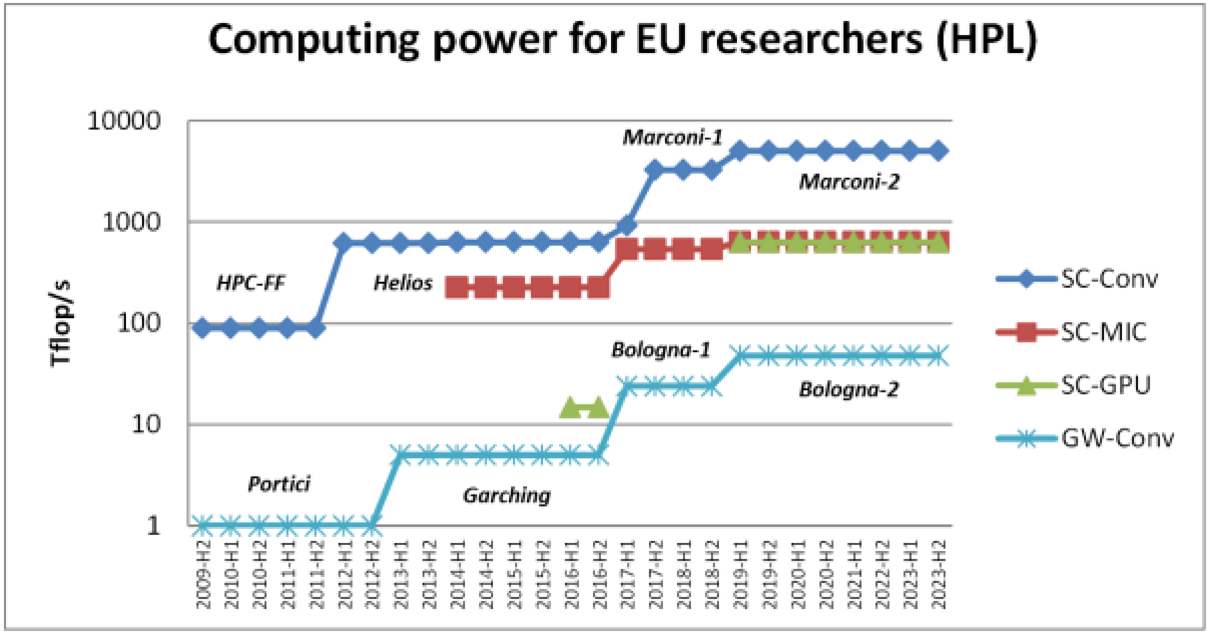
From the ITER research plan -2018 - (ITR-18-003)

- "It is very important that these **experimental studies are accompanied by a substantial effort in the simulation of ITER operational scenarios.** Present day devices will never be capable to fully emulate ITER operational scenarios, but they can **validate individual models** that can be used for the predictive simulation of such scenarios"

- **"ITER operation is expensive** and any component damage resulting from operational errors can potentially lead to high **repair costs and significant downtime** of the facility. Hence **predictive simulations,** using the ITER integrated modelling platform (IMAS), to assess plasma control, develop operation scenarios and prepare experiments**, will be essential for reliable and efficient ITER operation**"

Computing Resources for large scale simulation and integrated modeling

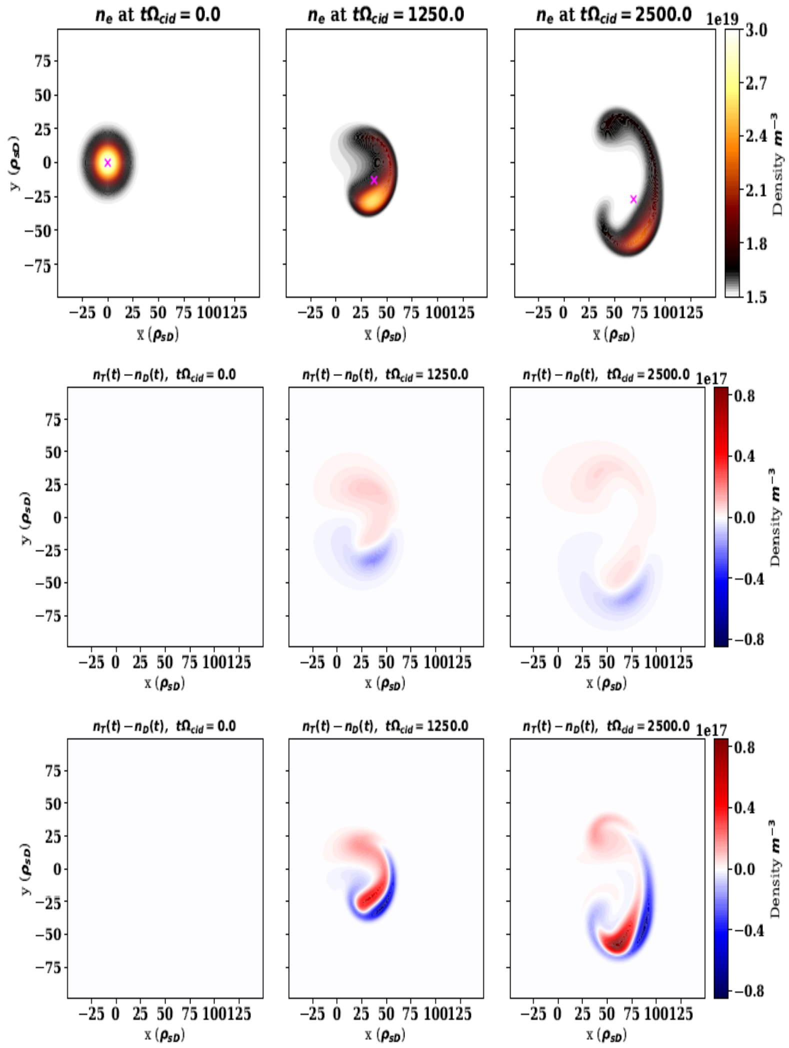
- **Steady evolution over the last 20 years (around x10 every 5 years)**



- **Expert group to assess the needs of EU fusion community in terms of HPC**
  - EUROfusion-dedicated HPC resources should be procured (medium size systems)
  - a vigorous effort in high level support for code development
  - EUROfusion should liaise with EuroHPC (extreme computing needs)

Challenge 2: integrate relevant physics

- Need to **integrate additional physics in turbulence models** for consistent environment
  - E.g.: **neutrals**, **impurities**…
  - Poses specific numerical challenges in 3D turbulent framework



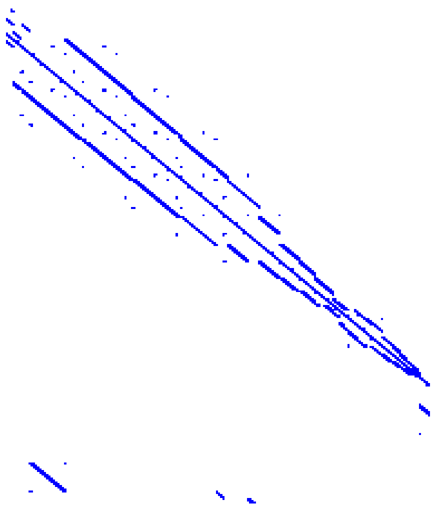
- E.g. of **multi-species gyro-fluid models**:
  - **Proof of principle established** in FELTOR code (MIHESEL mode) based on Zhdanov closure *[A. Poulsen, PoP 27, 032305 (2020)]*
  - Will be challenging to scale up to 3D reactor simulations ➔ research needed

Challenge 3: optimize codes for HPC

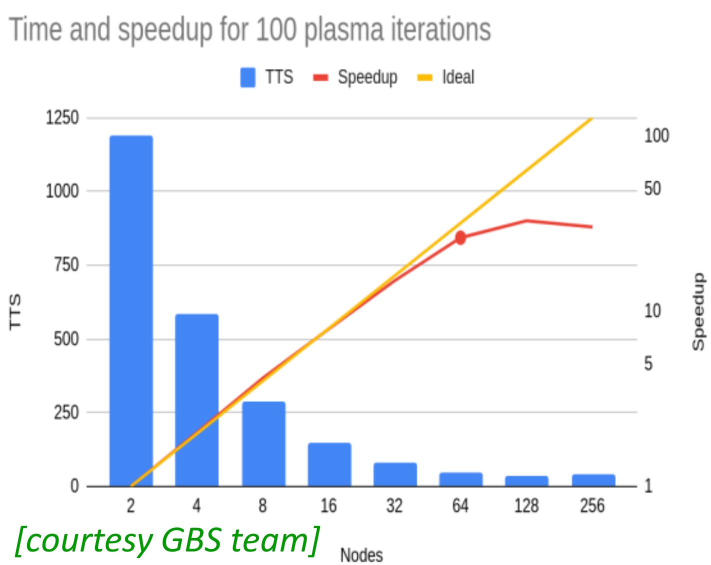
- 2 objectives:
  1. Reduce time for given case (strong scaling)
  2. Unlock applications to larger machines (weak scaling)

- In Pilot Phase, focus on optimization of common bottleneck of existing codes = **elliptic solvers** for plasma potentials
  - Large margin for progress illustrated by tests on GBS code (use of PETSC and GPUs)

- Activity expected to **scale up with the deployment of ACH**
  - Pilot Phase: **0.5ppy/year** ➔ 2021-2023: **2.25ppy/year**



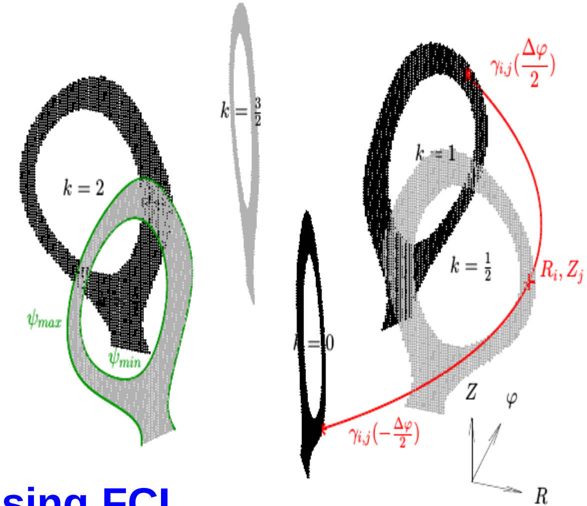
Matrix structure from ES potential solver in TOKAM3X diverted case



[courtesy GBS team]

Challenge 4: reduce algorithmic intensity

- Advanced parallel discretization methods based on **Flux Coordinate Independent (FCI)** approach
  [Hariri, CPC 184 (2013), Stegmeir, CPC 198 (2016)]
  - Potential to **reduce strongly computational needs**
  - Open issues: non-aligned structures and boundary cond.



- Comparative **study in pilot phase** demonstrated:
  - For general (even non-aligned) structures **no drawback in using FCI**
  - FCI allows strong **reduction of computational needs** (mesh resolution and time step)

Scaling of computational cost of non-aligned scheme vs. FCI: **$R_0 / (q\rho_s) \sim 5\times10^9$ for DEMO**

[Stegmeir et al., report, https://users.euro-fusion.org/iterphysicswiki/images/a/aa/Parallel_Discretization.pdf, (2020)]

- Remaining **challenges** for next project phase:
  - Treatment of **boundary conditions within FCI** → Immersed boundary technique
  - Extension to finite element methods

Develop high-potential numerical methods

- Special focus of Pilot Phase: **Hybrid Discontinuous Galerkin** (HDG) approach
  - pros: magnetic/wall **geometrical flexibility**, **high order** easily achievable (p/h-adaptivity), **reduces DOF** of global implicit systems
  - cons: complex, relatively novel in fusion

- An **HDG edge plasma solver** currently being developed by a team of ~6 developers in 4 labs
  - First release expected early 2021 (2D turbulence with neutrals) *[https://gitlab.mpcdf.mpg.de/stegmeia/etascebc]*
  - Upstream demonstration of potential of method on **2D/3D mean-field cases in full geometry** and **turbulence cases in reduced geometry**