How to keep up with fast-ions: the technical part

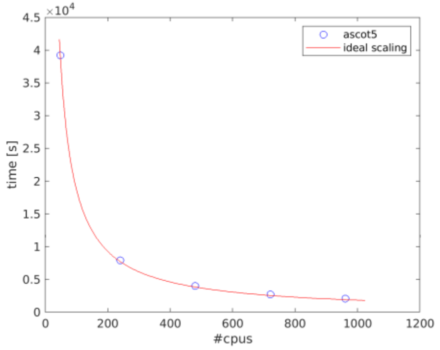
A. Snicker **et al.**

-Numerical models in nutshell
-Comparing typical runs
-Newest new: ASCOT-BMC, ASCOT-GPU
-Code development: git, slack, community

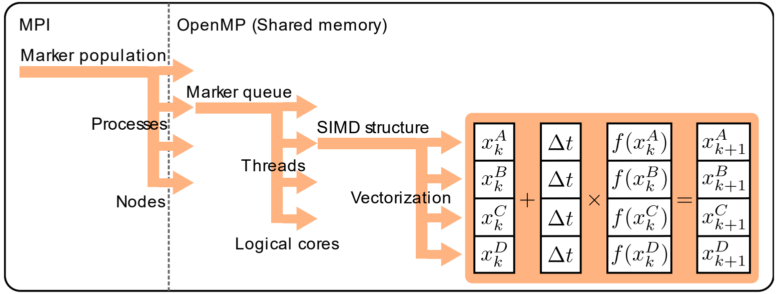
A. Snicker et al.

Numerical models, of HPC relevance 1/2

- ASCOT is a Monte Carlo orbit-following code
  - For minority species (like fast-ions)
  - No self-interactions
  - Coulomb collisions with background plasma
  - Near embarrassingly parallel using MPI/MPI+OpenMP
- Several layers of parallelism available in ASCOT5
  - Marker ensemble -> MPI
  - Marker queue -> OpenMP
  - Vectorization -> SIMD



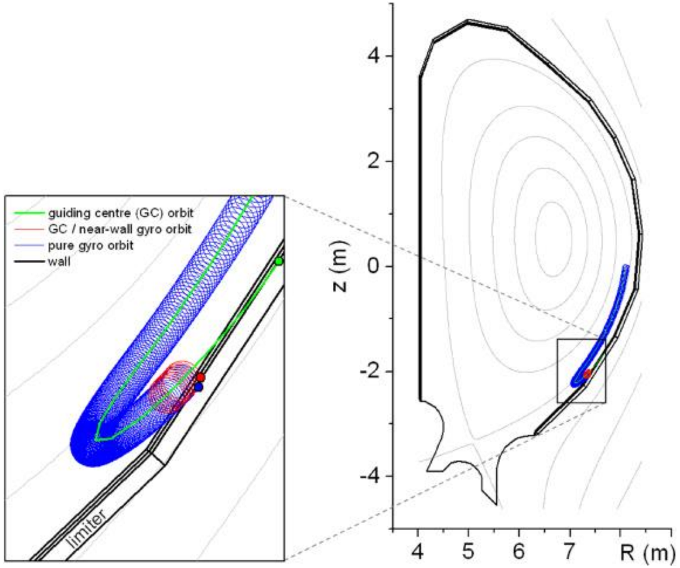
Scalability test of ASCOT5 with the number of CPUs in MARCONI



10 x 48 8 = 3840

Numerical models, of HPC relevance 2/2

- Guiding center vs. gyro motion [1]
  - For most applications GC is fine
  - But GC approximation does fail, e.g. [2]
- Running with gyro motion comes with cost
  - Roughly 30-100 times more CPU hours
- Typical tokamak run with 2D axisymmetric field
  - ~30 core hours (100k markers)
- Typical stellarator run with 3D field
  - ~300 core hours (100k markers)
- Additional considerations:
  - Alfven eigenmodes [3] – 1D spline per mode
  - ICRH via RFOF operator – two-stage simulation process [4]



[1] A. Snicker *et al* 2012 *Nucl. Fusion* **52** 094011

[2] A. Sperduti *et al* 2021 *Nucl. Fusion* **61** 016028, A Sperduti *et al* 2021 *Plasma Phys. Control. Fusion* **63** 015015, P Ollus *et al* 2022 *Plasma Phys. Control. Fusion* **64** 035014

[3] A. Snicker *et al* 2013 *Nucl. Fusion* **53** 093028

[4] S. Sipilä *et al* 2021 *Nucl. Fusion* **61** 086026

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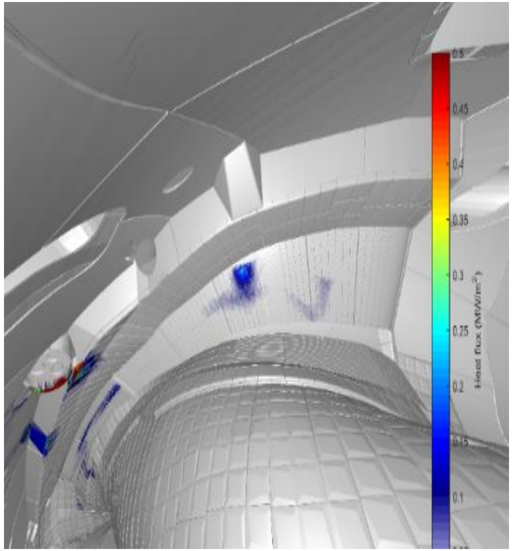
A. Snicker et al.

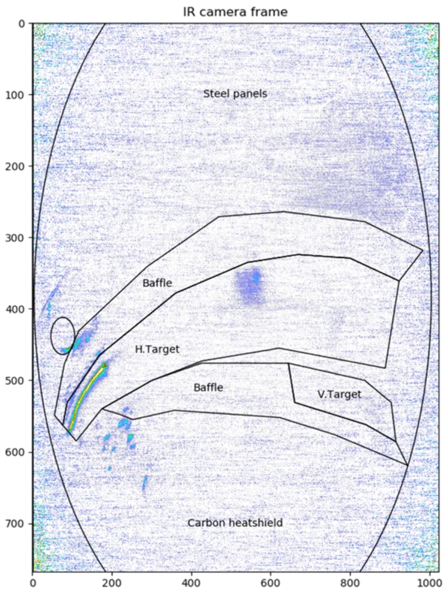
ASCOT simulations showcases

- W7-X wall power load high-definition
  - Example of complex 3D geometry and useful validation
- ASCOT-RFOF for AUG
  - Example of the added CPU demands by IC operator
- ITER FILD simulations
  - Example of the intrinsic Monte Carlo statistics problem

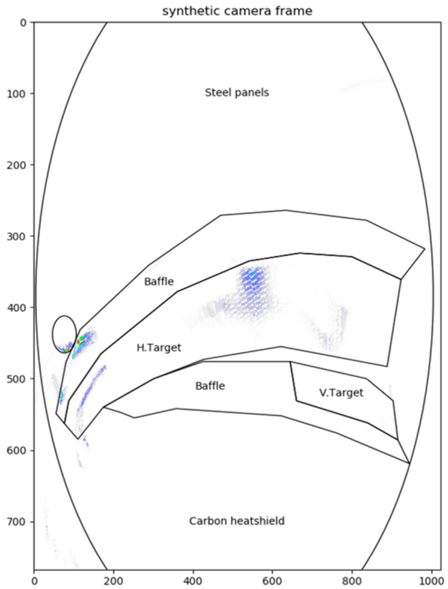
Synthetic IR studies with ASCOT (in W7-X)



ASCOT'S view of W7-X intestines



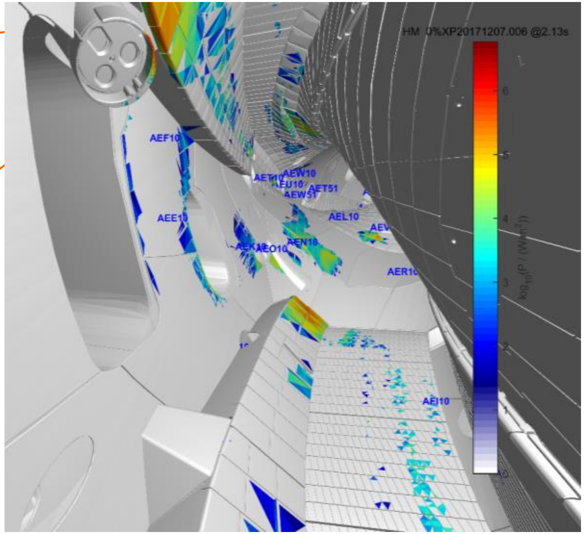
InfraRed (IR) camera frame of the same place

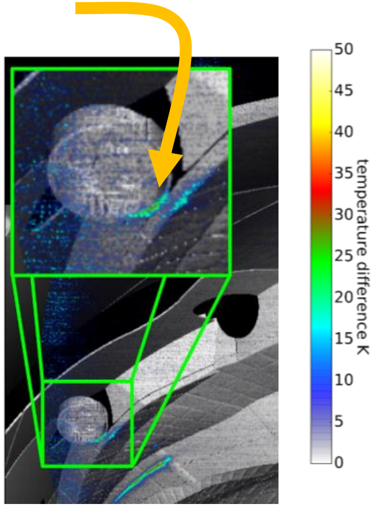


ASCOT's synthetic IR camera frame

Wall design improved thanks to ASCOT simulations !

Fragile (sapphire) vacuum windows





ASCOT predicted excessive NBI power loads
➔
Protective collar installed before starting the beams

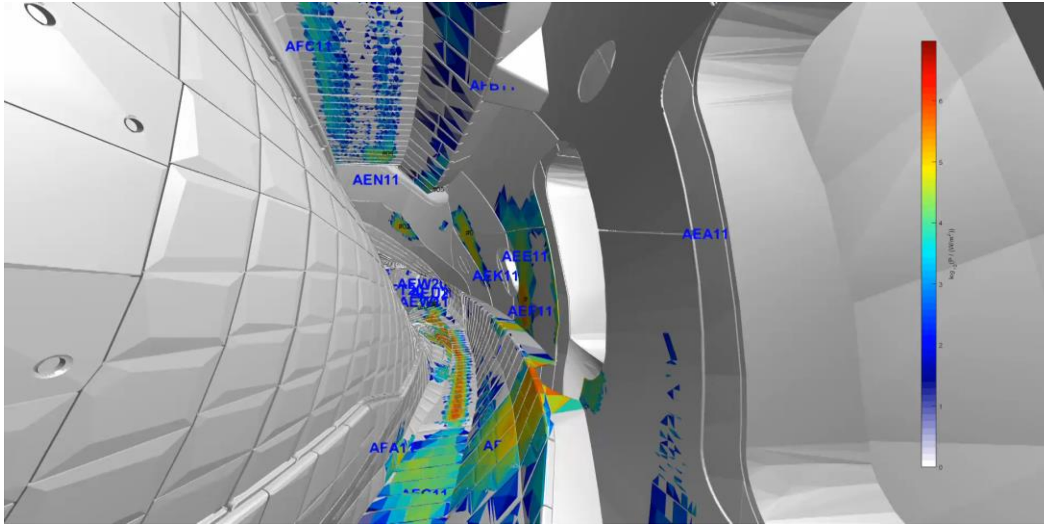
Wendelstein 7-X á l'ASCOT

power loads in excess of 1.5MW/m^2 measured

[5] S. Äkäslompolo Fusion Eng. and Des. 2019, **146**, 862; S. Äkäslompolo et al 2018 Nucl. Fusion 58 082010

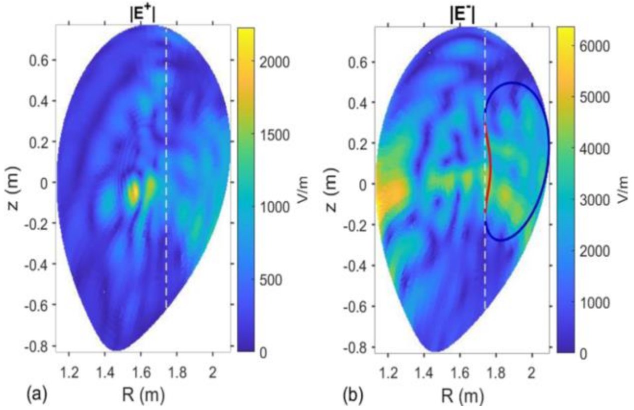
Simulation specifications

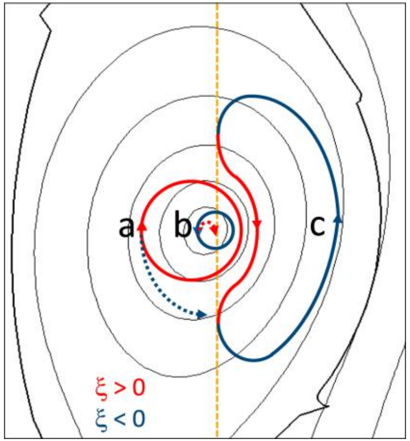
- 1M-100M GC markers
  - Converged peak heat load (100M)
  - Hot spots and estimated peaks (1M)
- CAD 3D wall, ~4M triangles
  - Triangle areas 1 mm^2 to 0.2 m^2
- Simulation was MARCONI commissioning
- Estimated CPU hours: 300k



AUG-RFOF synthetic FILD

- Simulate ICRH-heated fast-ions
  - Both NBI and minority ions absorb IC power
  - Synthetic FILD vs. measured FILD
- Two-staged simulation process
  - Run with MC RFOF operator
  - Obtain the steady-state distribution function
  - Marker sampling for synthetic FILD simulation
- Improved statistics for the synthetic FILD





[6] S. Sipilä *et al* 2021 *Nucl. Fusion* **61** 086026

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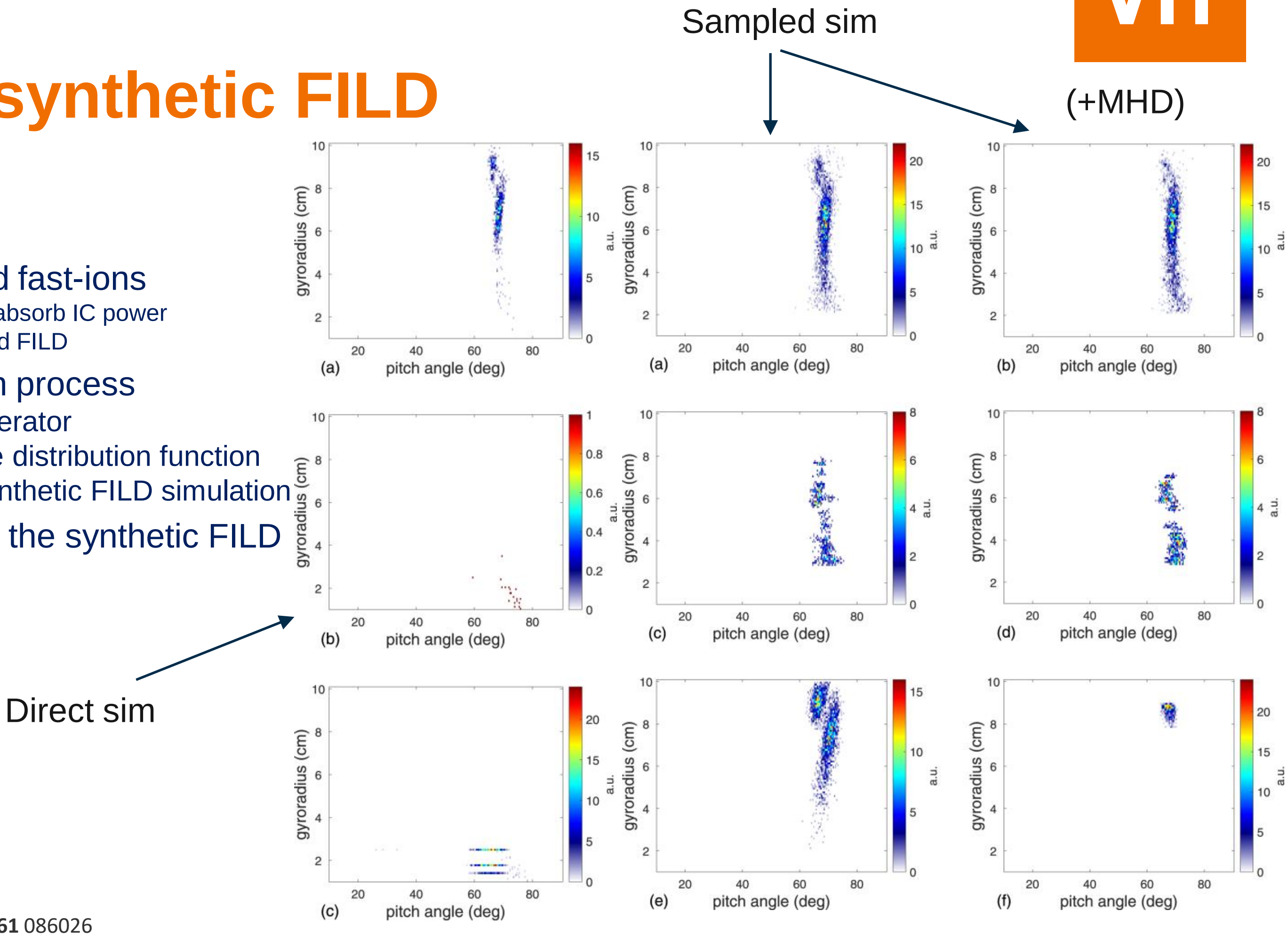

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  - Obtain the steady-state distribution function
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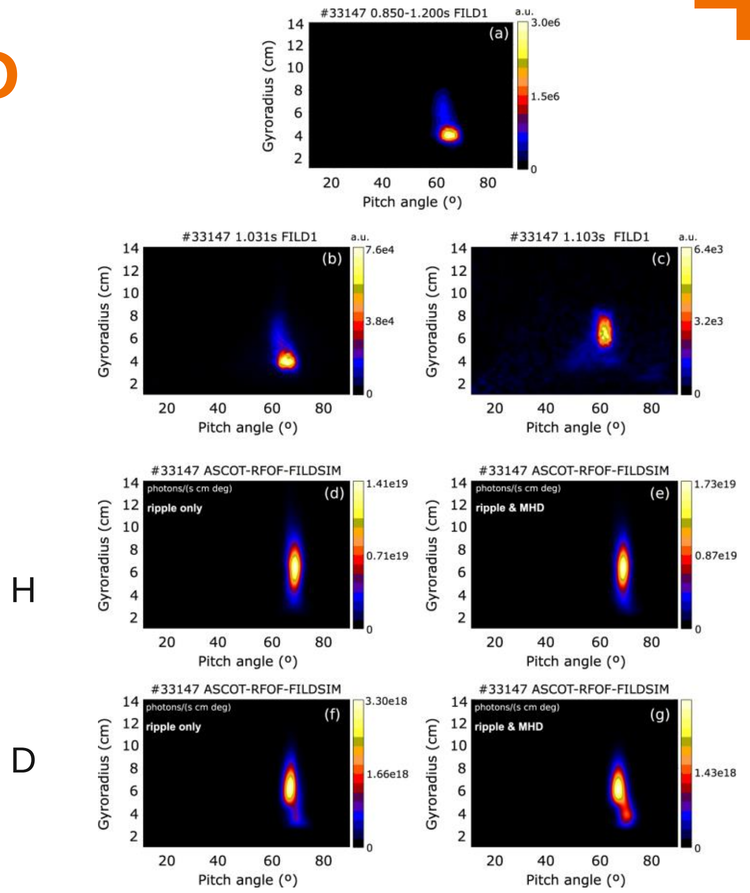
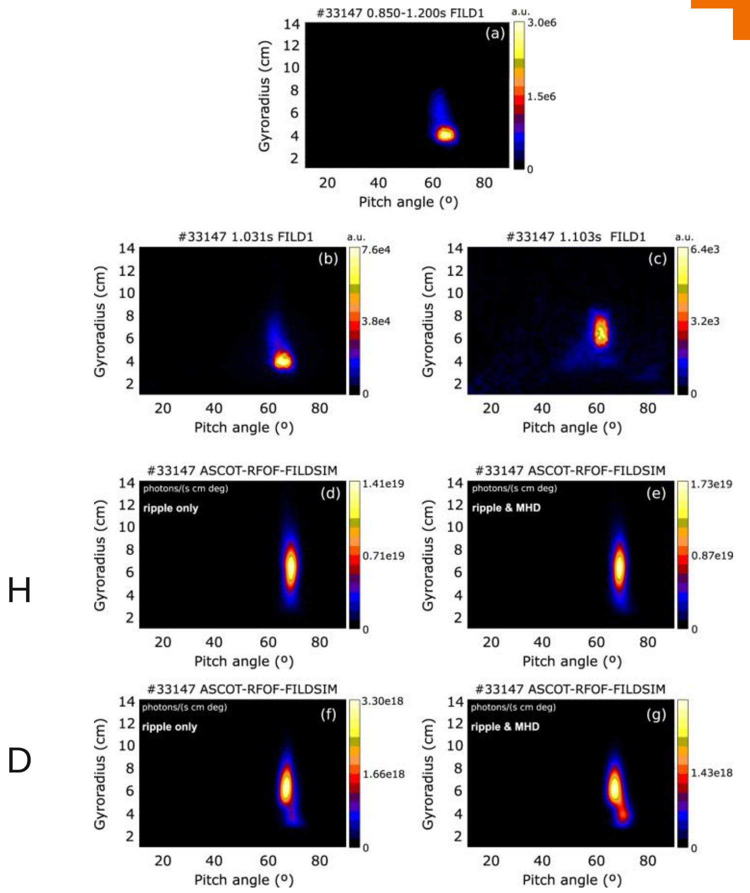
- Improved statistics for the synthetic FILD
  - Questions remain:
    - What is the actual H population?
    - Why the H tail is simulated higher?



[6] S. Sipilä *et al* 2021 *Nucl. Fusion* **61** 086026

Simulation specifications

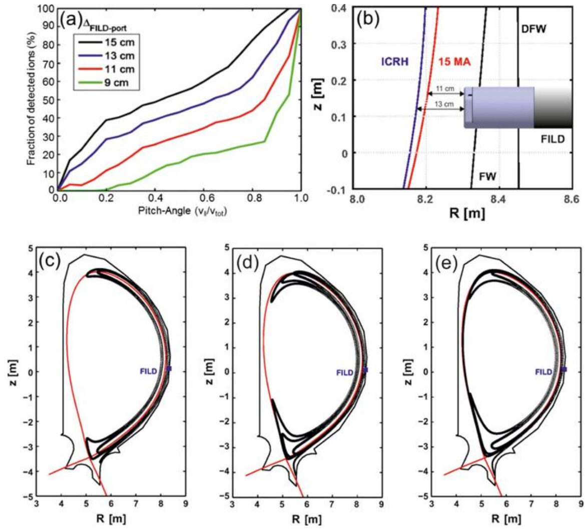
- 200k-500k GC markers
  - With MHD 200k, without 500k
  - Sampling: 3k FILD hits=~38M markers
- Simulations in MARCONI fusion
- CPU costs:
  - Heating simulation for H, 55k CPUh
  - FILD simulation for H, 3k CPUh
  - From above: MHD cost=factor of 2.5

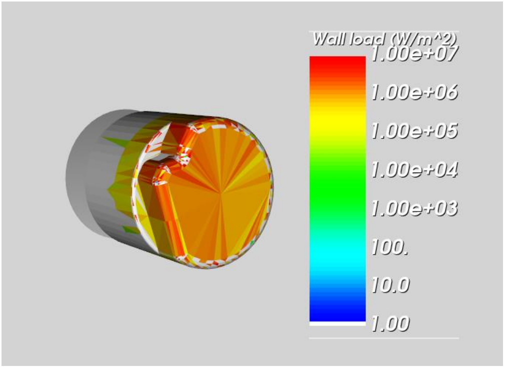


[6] S. Sipilä *et al* 2021 *Nucl. Fusion* **61** 086026

ITER FILD simulations

- Goal: simulate synthetic signal using ASCOT+FILDSIM
- Intrinsic issue: poor statistics of narrow-escape
  - First wall 600? m^2, FILD head 413 cm^2, the pinhole 1 cm^2
  - Likelihood to hit pinhole (dummy math) 1/10M!!!
- Solution for production runs:
  - Brute-force
  - Running maximum number of markers
- Practical implication:
  - Scans for various scenarios, pinhole geometries etc.
  - Only use high statistics when needed
- Can we do better?
  - What if we could start our simulation from the pinhole…





[8] M. Garcia-Munoz et al. *Rev. Sci. Instrum.* 87, 11D829 (2016)
[9] X. Litaudon, submitted to Nuclear Fusion 2023

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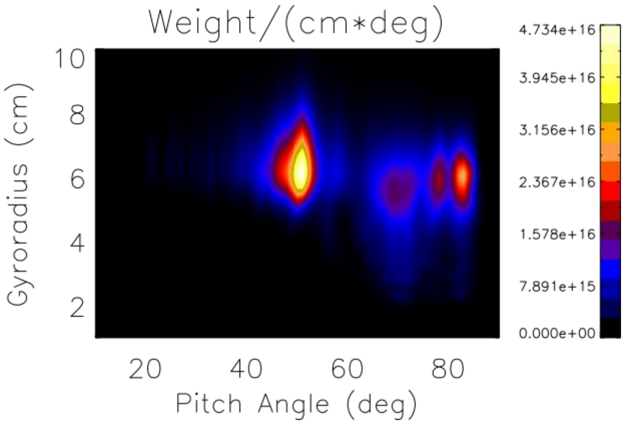
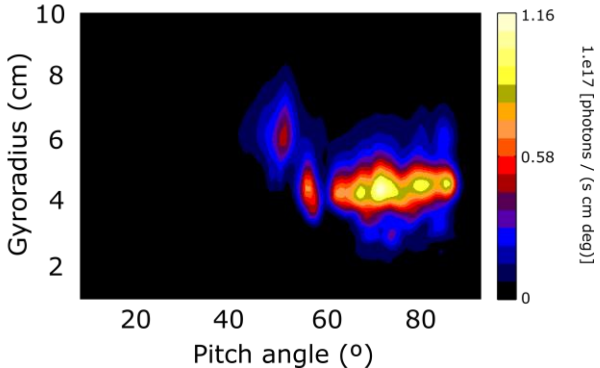
alphas



alphas+beam ions



[9] X. Litaudon, submitted to Nuclear Fusion 2023

ACADEMY OF FINLAND

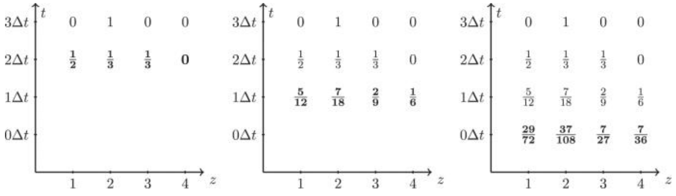
VTT

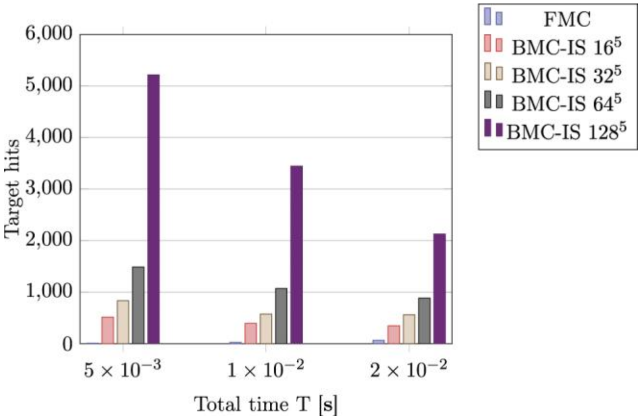
-Numerical models in nutshell
-Comparing typical runs
-Newest new: ASCOT-BMC, ASCOT-GPU
-Code development: git, slack, community

A. Snicker et al.

Backwards Monte Carlo

- Instead of brute force, use math and computers
- Iterative equations for probability distribution in phase-space
  - Allows to calculate the likelihood for marker from phase-space to the pinhole
  - Use known birth distribution, convolution of the two will give you a signal
  - Plan B adopted in this publication: use the likelihood to importance sample
- The efficiency increase by a factor of 10-100

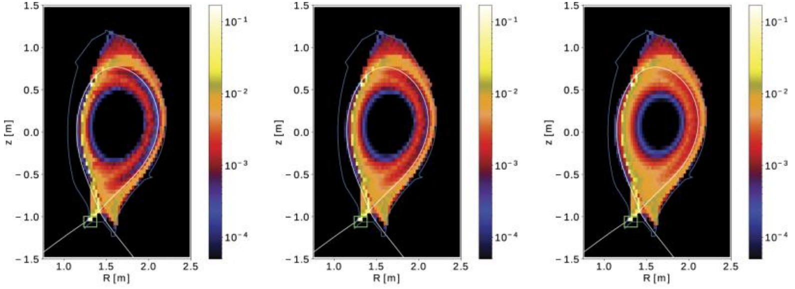




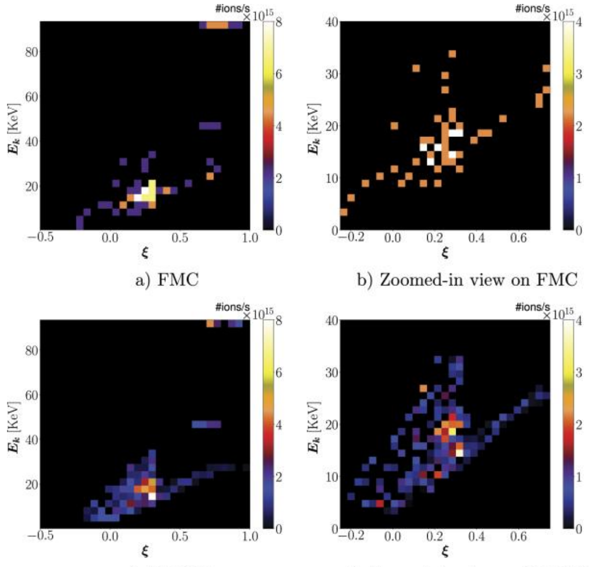
[10] F. Zonta *et al* 2022 *Nucl. Fusion* **62** 026010

Backwards Monte Carlo

- Instead of brute force, use math and computers
- Iterative equations for probability distribution in phase-space
  - Allows to calculate the likelihood for marker in all phase-space to the pinhole
  - Use known birth distribution, convolution of the two will give you a signal
  - Plan B adopted in this publication: use the likelihood to importance sample
- The efficiency increase by a factor of 10-100
- Shown to reproduce forward model results
- Caveats:
  - Using 2D wall, 3D wall turns to be a nightmare…



a) BMC, $T = 5 \times 10^{-3}$s b) BMC, $T = 1 \times 10^{-2}$s c) BMC, $T = 2 \times 10^{-2}$s



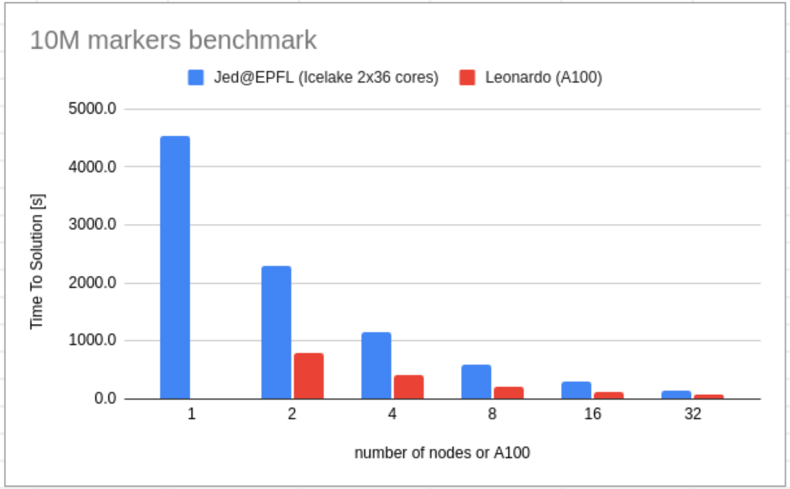
a) FMC b) Zoomed-in view on FMC

c) BMC-IS d) Zoomed-in view on BMC-IS

[10] F. Zonta *et al* 2022 *Nucl. Fusion* **62** 026010

ASCOT GPU

- Originally, ASCOT developed for Xeon Phi
- Can we directly use the same parallelism for GPU?
- How efficient the code will be?
- More details were given earlier today by G. Fourestey
- Next steps:
  - Check that the 3D wall and collisions work
  - Merge to main development branch
  - Try production runs?



-Numerical models in nutshell
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A. Snicker et al.

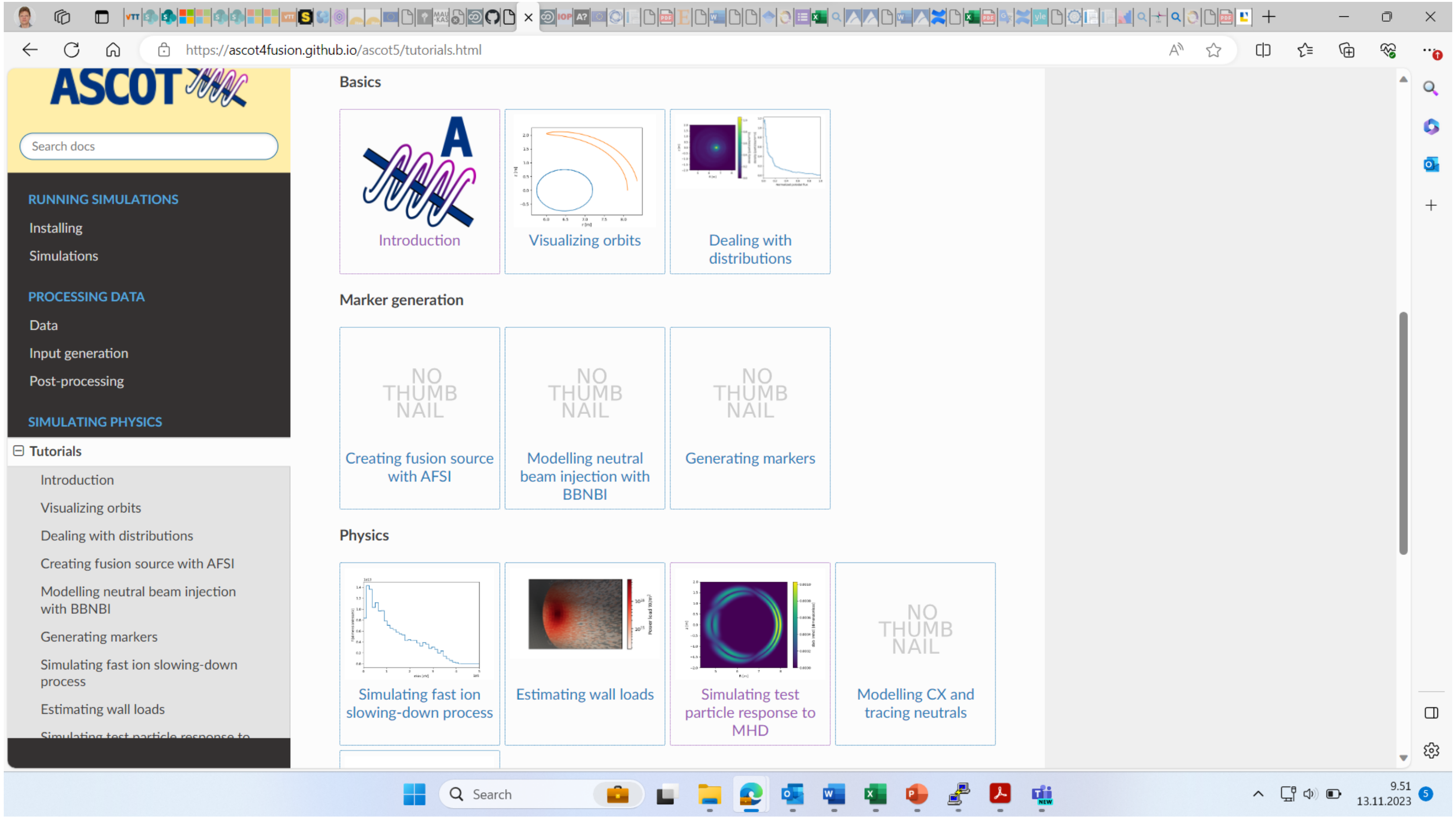
Ideology of constant development

- Adopting from fission, we need to constantly adapt
  - New supercomputers (the algorithms might not be efficient), e.g. GPU
  - New physics introduced (the code skeleton based on known physics), e.g. ICRH
  - Constant need to adapt to these!
- ASCOT has been built from the scratch twice, during last 10 years
  - ASCOT4 in FORTRAN and MPI around 2013
  - ASCOT5 in C and MPI/OpenMP around 2017
- A large userbase:
  - A set of tutorials to ease the onboarding process
  - Manuals and videos helping
  - Slack and weekly meetings

A new home for the ASCOT - github

- Since October 2023, ASCOT moved to open-source licensing
  - Code is operated under LGPL 3.0 license
  - Currently building the user community there
- Structure of the github:
  - Main branch always stable – only pull requests accepted, tags for new releases
  - Hotfixes done under main
  - Develop open for, well, developers
    - Developers can push, others still need pull request
    - New features under develop in a separate branch
  - Automated testing processes
    - Each push -> testing compilation+fast unit tests (~5min)
    - Pushing to develop -> above + physics tests+tutorials+documentation (~1h)
    - Pull request to main -> above + regression tests (WIP) (~a few days)
    - Each test can be run on will
  - Tutorials and documentation within github

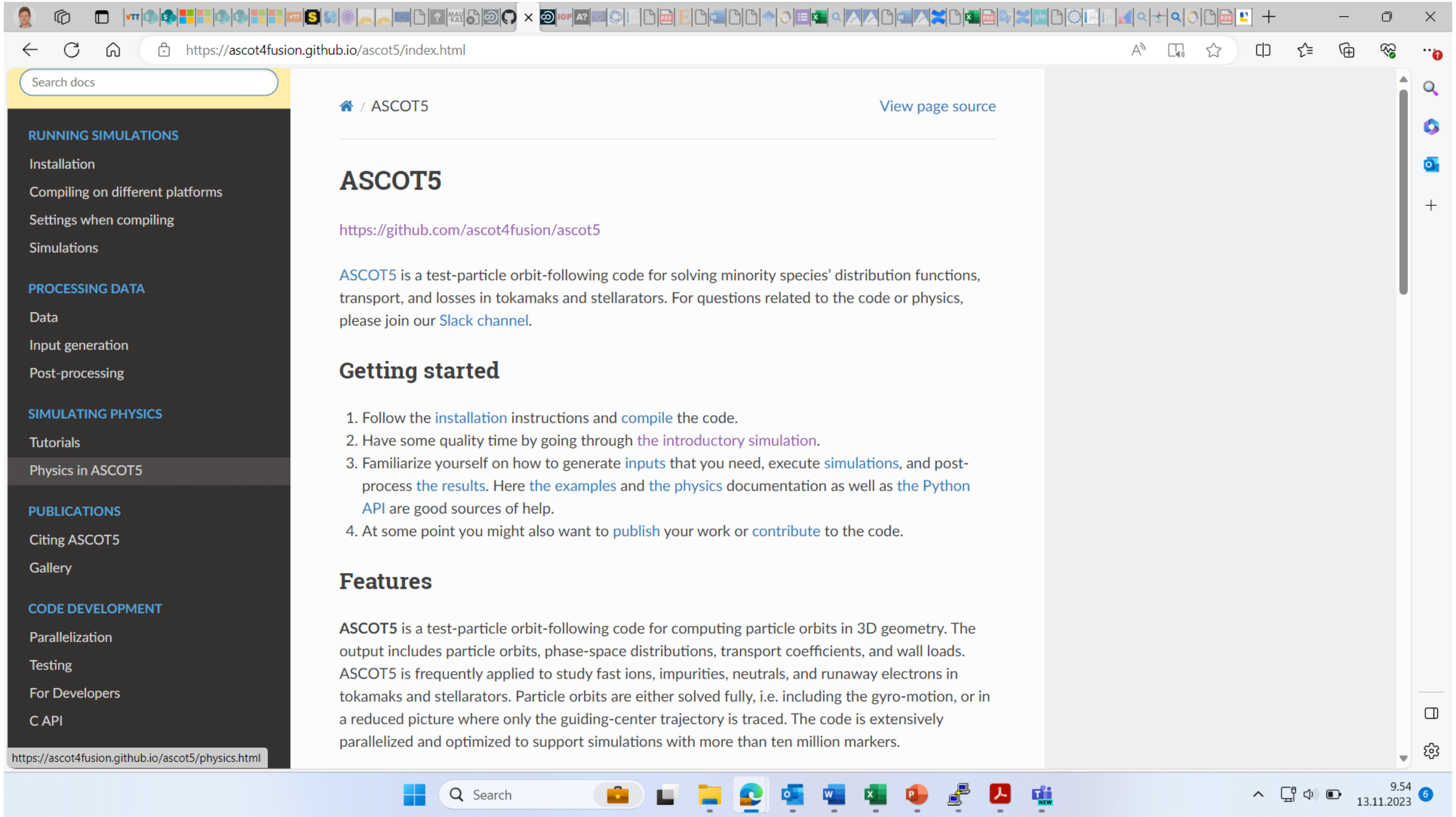
Tutorials within the github - notebooks



VTT

Tutorials within the github - notebooks

Documentation within github



Building the user community

- EUROfusion funded training camps
  - 1st was organized in 2019 (~12 participants)
  - 2nd last week (~25 participants)
- ASCOT is a global project
  - West (Europe, US) and EAST (China)
  - North (Finland)
  - Need some users from Australia or from South-America to cover global South, anyone?
- Casual discussions using slack
- Weekly meetings via zoom

Building the user community

beyond
the obvious

A. Snicker

How to keep up with fast ions in the increasingly complex fusion devices?

Taina Kurki-Suonio & Antti Snicker
Aalto University & VTT

Contents

- ★ What are the ***fast ions*** in fusion world?
- ★ Going from pen&paper to simulations requiring supercomputing
  - – Axisymmetric, circular plasmas (from pen&paper to analytical models)
  - – Real-life tokamaks: introduce a variety of mechanism breaking the axisymmetry
    - The ultimate case: *stellarator*
  - – Make contact with the outside world: introduce SOL and the 3D wall structures
  - – Accurate power distributions on the first wall: from GC following to resolving gyro orbits
  - – Realistic (non-quiescent) plasmas: introduce NTMs, TAEs, turbulence …

Fast ion in fusion devices

- ★ The fusion plasma as a whole is hot, >10 keV
- ★ To keep it hot, we need to have particles with even higher energies that collisionally heat the fuel plasma to compensate for the inevitable losses'

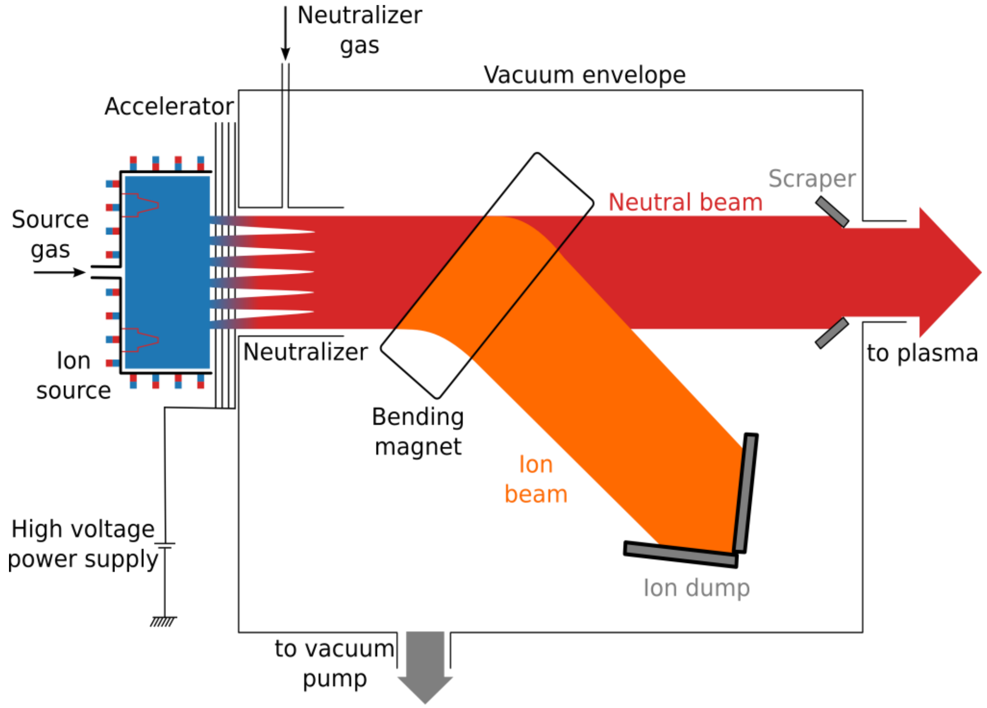
These particles are the ***fast ions***

- ★ In today's devices, fast ions are generated externally

- ★ In a fusion reactor, the fast ions are generated by the fusion reactions themselves, and the fusion conditions are self-sustained …

Generating fast ions externally

- ★ ICRH ➔ minority ions in MeV range
- ★ Neutral beams:
  - – PNBI ➔ D (~100 keV)
  - – NNBI ➔ D (~1 MeV)

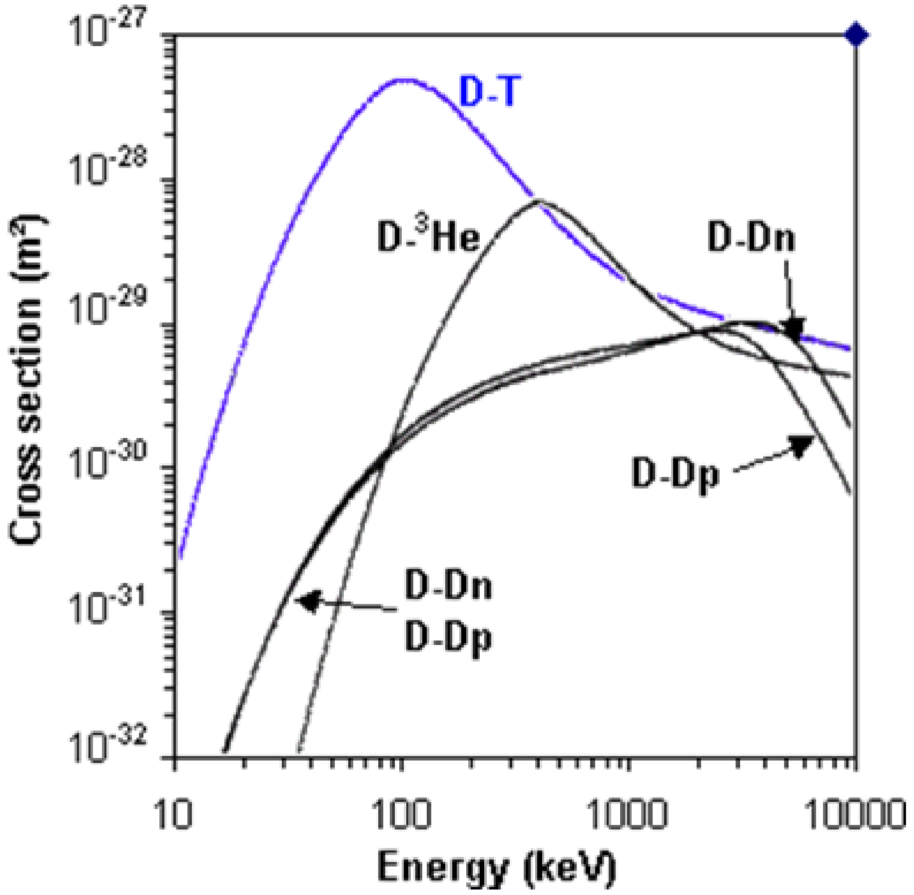


JET ITER-like antenna

Fast ions from fusion reactions

★ α's, p's, T's & ^{3}He's in MeV range from fusion reactions – now and in the future:

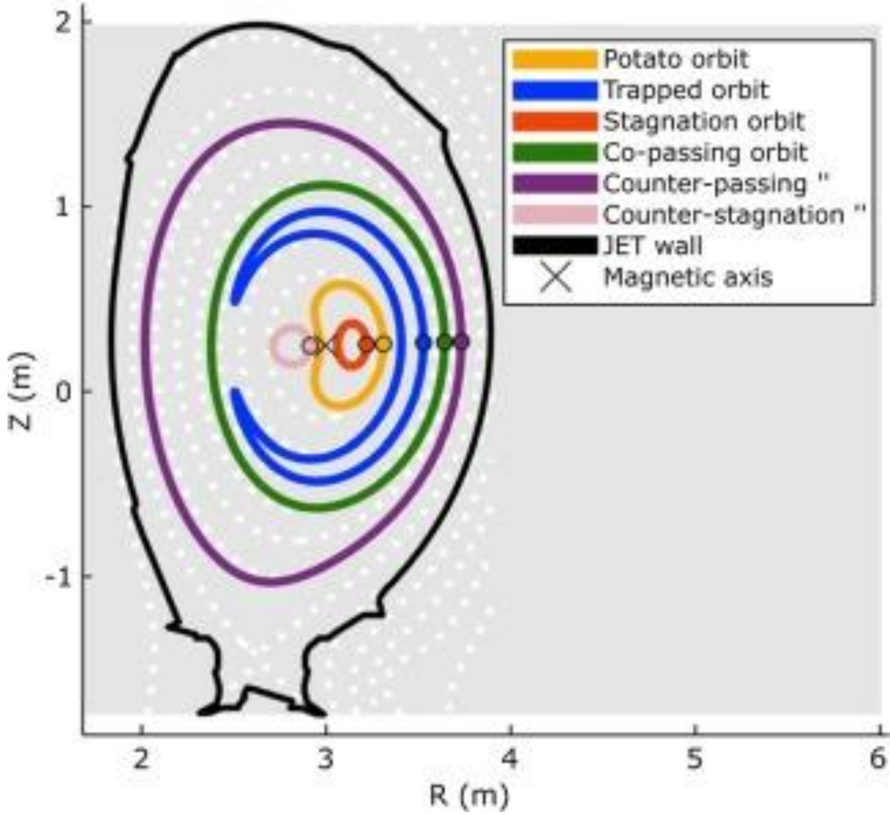
- D + D ➔ ^{3}He (0.8 MeV) + n (2.45 MeV)
- D + D ➔ T (1 MeV) + p (3 MeV)
- D + T ➔ α (3.5 MeV) + n (14.1 MeV)
- ^{3}He + D ➔ α (3.6 MeV) + n (14.7 MeV)



Confining fast ions

Axisymmetric tokamak

- ★ ’perfect’ confinement
  - – Mathematically quaranteed: according to *Noether’s theorem* any symmetry is associated with a constant of motion
  - – In axisymmetric tokamak this is the *toroidal canonical momentum*
  - – Axisymmetry ensures that the particle *drift orbits* close upon themselves and do not wander radially
- ★ Only Coulomb collisions slowly kick the ions outward



Benjamin et al., Computer Physics Communications 292 (2023) 108893

Simulating fast ions in axisymmetric tokamak…

… is very easy and fast!

★ The toroidal magnetic geometry can be expressed *analytically*

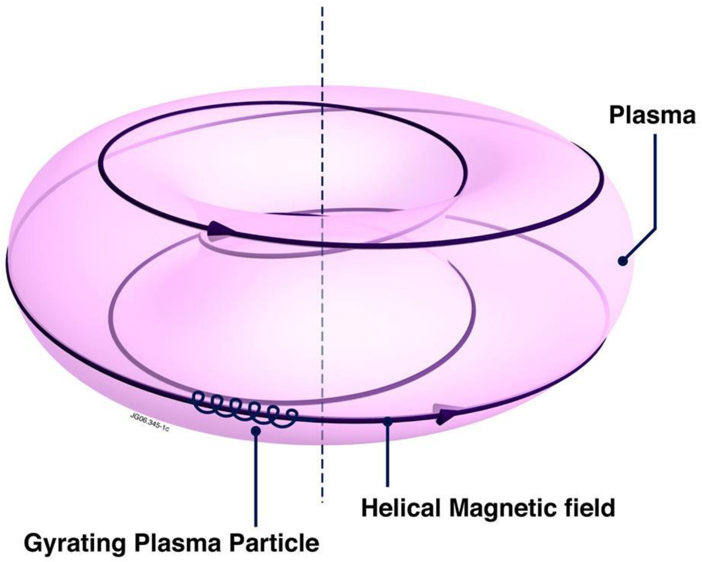
- *No numerical divergence*
- *No need for interpolations*

★ One can use *field-aligned flux coordinates* in following par

- *Long time steps allowed ➔ Integrating equations of motion for the guiding-centers is very fast*

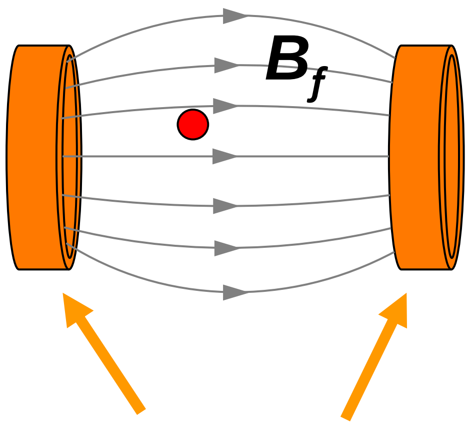
★ This approach (ASCOT 1.0 and 2.0) was ok for assessing the zeroth-order effects due to Coulomb collisions:

- particle ”confinement” (staying inside separatrix)
- power deposition



Real tokamaks and real needs, culminating to stellarators…

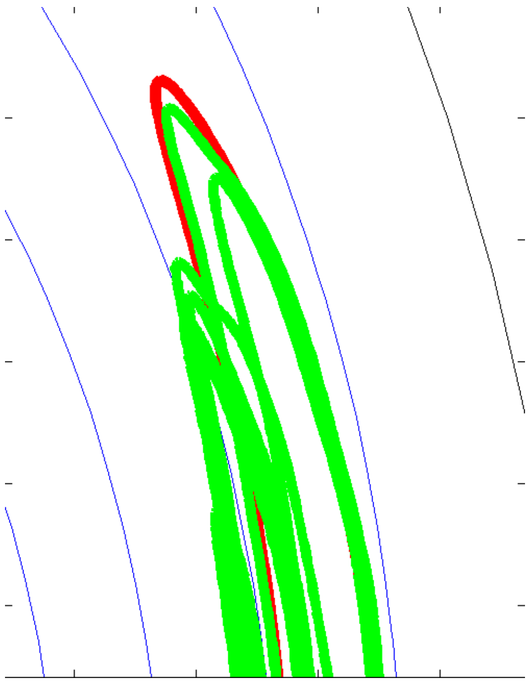
The axisymmetry is broken: Finite number of coils with finite size …



2 of the TF coils

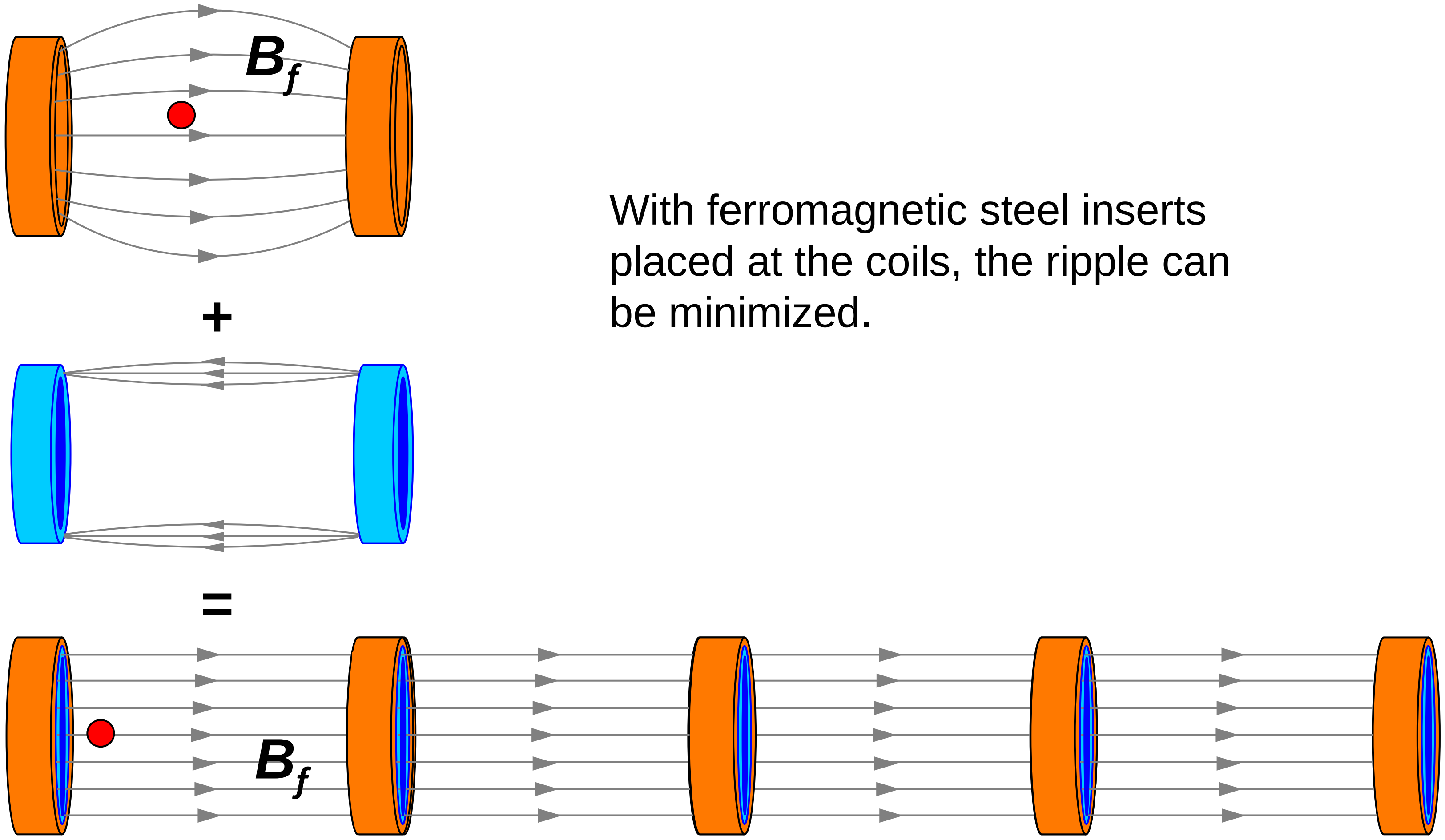
A finite number of TF coils
→ non-axisymmetric field, ***toroidal magnetic ripple***

The local magnetic "bottle" between two TF coils can trap charged particles, which quickly drift out of the plasma due to vertical grad-B drift.



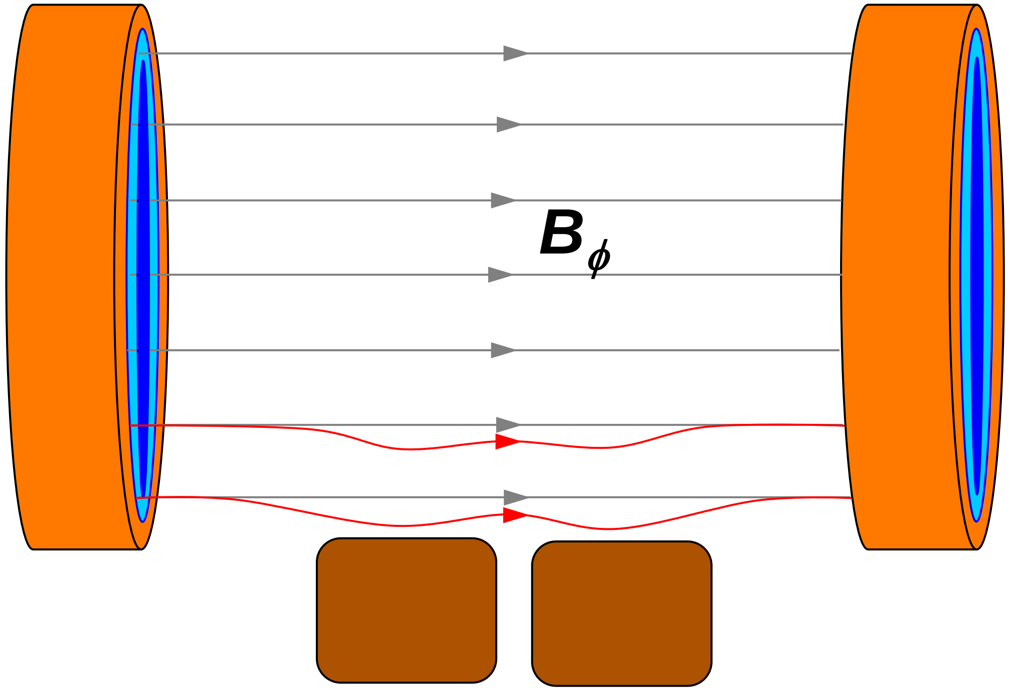
Banana orbits are no longer guaranteed to close in the poloidal plane and can start wandering even without collisions …

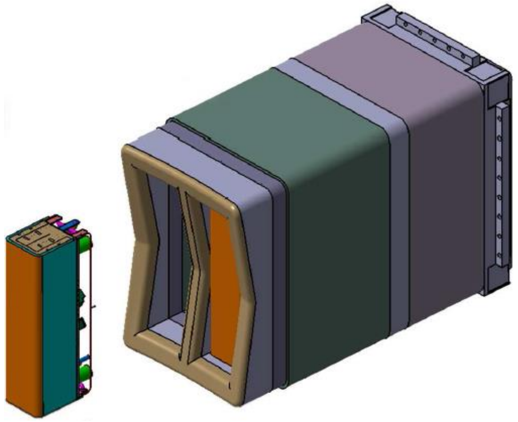
Trying to fix the broken symmetry: *ferritic inserts*



With ferromagnetic steel inserts placed at the coils, the ripple can be minimized.

But that's not all, folks: *Test Blanket Modules (TBM)*





TBM's containing ferritic steel very close to the plasma are placed at three toroidal locations between TF coils

Let us count our symmetry breakers…

- ★ Finite # of TF coils ➔ TF ripple
- ★ Ferromagnetic components ➔ localized magnetic perturbations
- ★ TBM blocks (or any other material sucking in magnetic field)
- ★ External coils, such as ELM control coils ➔ stochastization of edge magnetic field

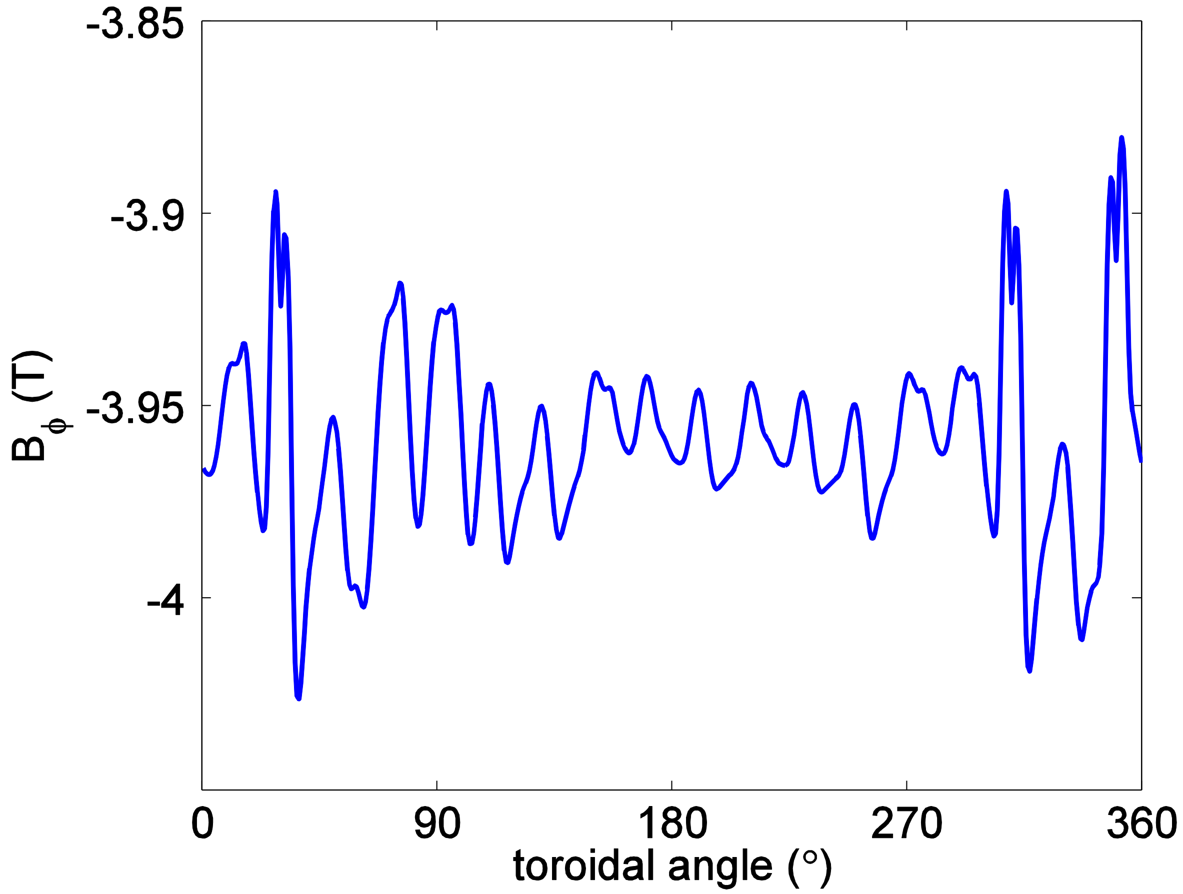
- ★ How does the total magnetic field look like?

B_T (φ) at the OMP separatrix in ITER 9MA Scenario

Toroidal ripple 1.1%,

Field bump due to NBI ports 0.57%

Field bump due to TBMs 1,1%



What are the implications to our simulations?

★ Need to tabulate the field & interpolate

➔ enormous increase in memory needs

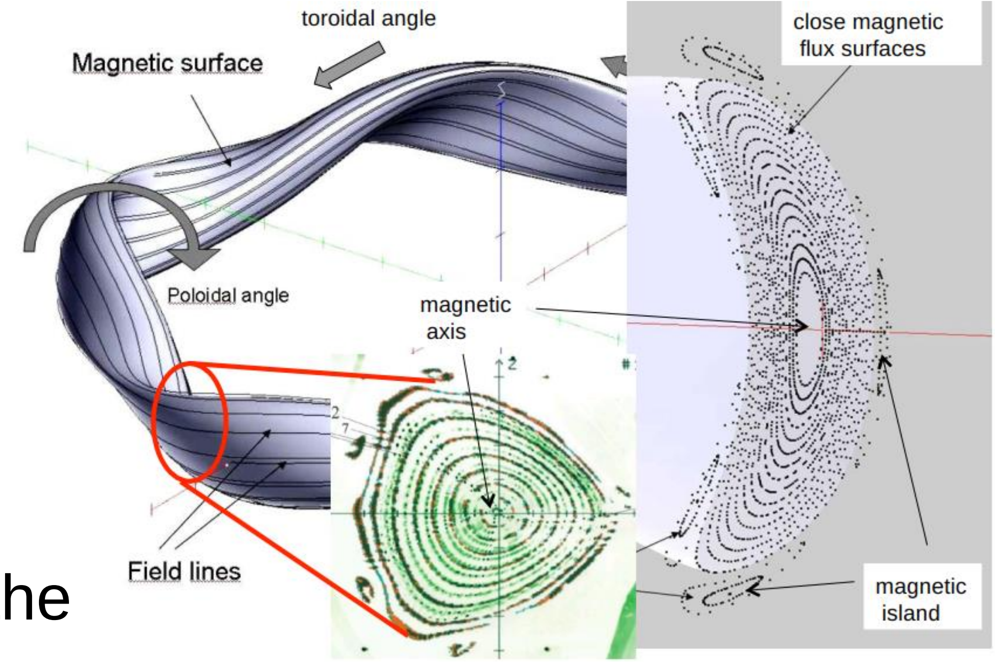
➔ good-bye kiss to field-aligned flux coordinates

➔ we have to keep a keen eye not to have

- Numerical divergence in the field
- Numerical drifts

★ Fine structures have to be seen and obeyed by the fast ions

➔ time step has to be shortened



Prime example of ultimate 3D features: *W7-X stellarator*

And as if that was not enough…

- ★ With a large number of fast ions (in ITER, fast ions account for about 1/3 of the total pressure), one has to worry about power loads to the first wall
  - – Both the peak power load evaluations and synthetic lost-ion diagnostics require a **high-fidelity first wall**
  - – For well-confined (= relevant plasmas), a very large particle ensemble is needed to yield **reasonable statistics** at the wall
  - ➔ parallelizations, vectorizationsy, GPUs…. (this is why ASCOT5 was born)
- ★ ASCOT only includes neoclassical physics, while real plasmas have much more character: *turbulence, NTMs, TAEs, …*

Including additional physics always has a computational cost – either in CPU/GPU time or memory consumption. Or both…

And now to Antti …