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Extreme Scale Computing with the Fusion Particle Code XGC1*†

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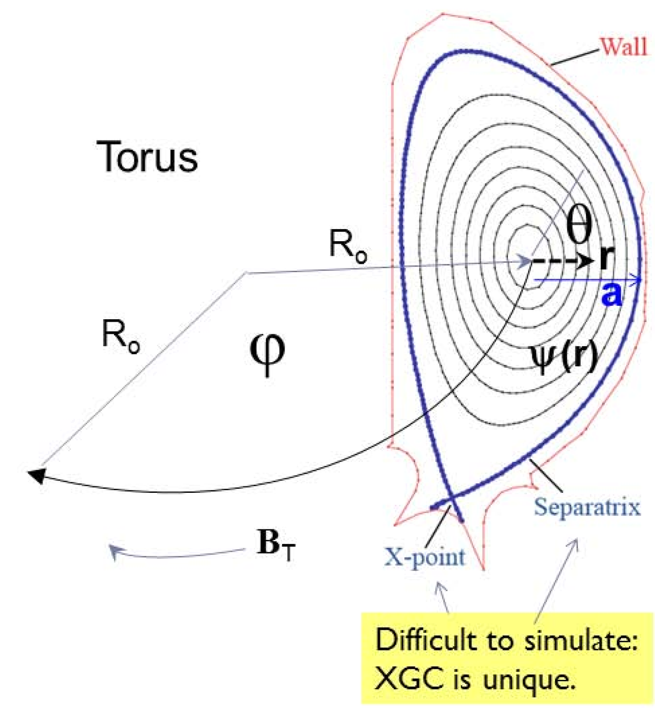
Introduction

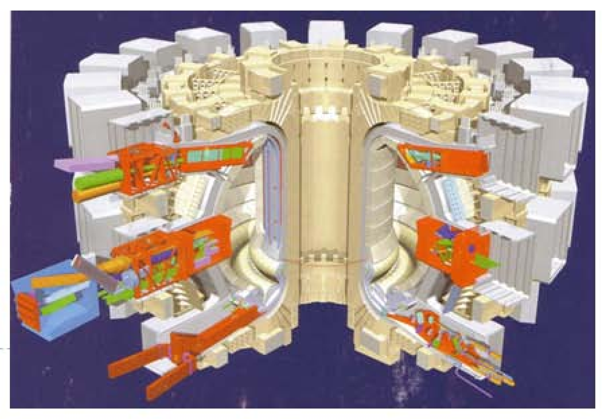
- Tokamak fusion plasma is a gaseous system of charged particles (D^+, T^+ and e^-), which flow along strong magnetic field lines in a torus (called magnetic confinement).
- When D^+ and T^+ ions are hot enough (>10 keV), they fuse together to form α particles (energetic He^{2+}) and release 14 MeV neutrons ($E=\Delta m c^2$).
- Energy from 14 MeV neutrons is used for electricity generation
- Tokamak plasma is subject to
  1. Collisional transport enhanced by inhomogeneous toroidal magnetic field (neoclassical transport)
  2. Micro-scale turbulences and slow loss of plasma
  3. Macro-scale instabilities and fast loss of plasma
- Assuming that the macro-scale instabilities (item 3) are controlled in a fusion reactor
  → **Our simulation is on item 1 and 2 in realistic diverted geometry.**

Tokamak geometry



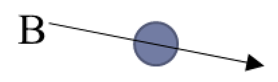
Poloidal cross-section (poloidal plane) at a constant toroidal angle

Poloidal magnetic flux label $\psi(r)$: 1 at r/a=1, 0 at r/a=0



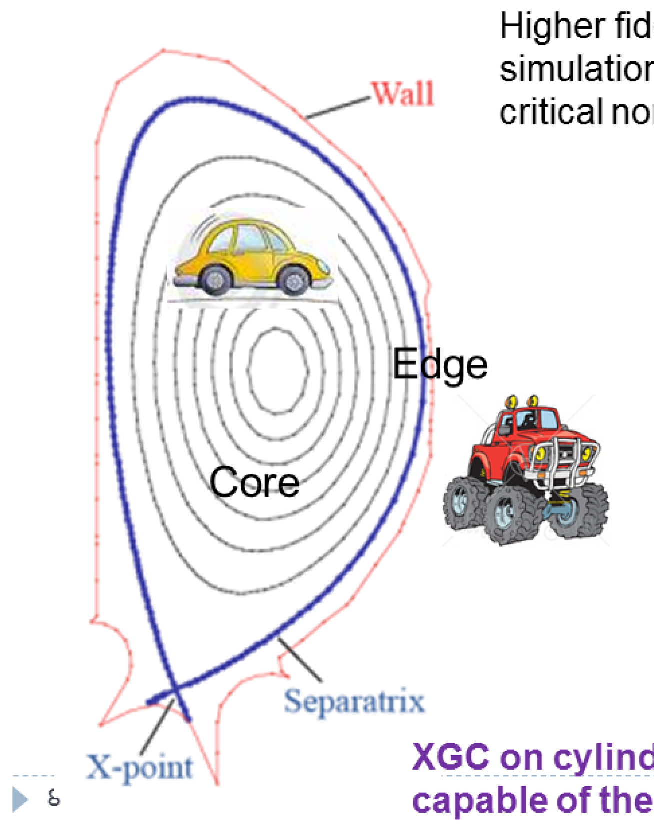
Gyrokinetic particle simulation of fusion plasma

- **Gyrokinetic:** Reduce 6D (x,y,z,v_1,v_2,v_3) to 5D ($x,y,z,v_{||},v_\perp$) by assuming that the gyrofrequency is much faster and that the gyroradius is much shorter than the interesting physics scale.



- **Particle-in-cell approach:** solve the marker particle dynamics in 5D space, and solve the Maxwell's equations on 3D position grid
  - Optimal for leadership-class computing (larger device or higher resolution physics → bigger grid→ more # particles → more # cores)
    - Because particle # per core is limited by memory size
  - Reduced memory requirement for higher v-space resolution via random v-space sampling
  - Statistical particle noise 1/Sqrt(N) → Smoothing or large enough N (convergence and sensitivity studies are needed)

Difficulty of the whole volume simulation



Higher fidelity physics needs whole volume simulation: many experimental evidences for critical non-local core-edge interactions.

Magnetic separatrix is a singular surface for core codes which use the easy-to-handle "magnetic" coordinate system.

Thus all the gyrokinetic codes stay in the core

- at a safe distance inside the magnetic separatrix surface.
- Delta-f is possible in the core.

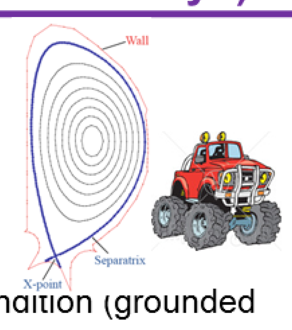
XGC on cylindrical grid is the only kinetic code capable of the whole-volume simulation.

Understanding the edge-core interaction is critical for fusion

- 30 years of experiments find that the edge plasma condition has a direct influence on the core fusion plasma condition
  - at a much faster information transmission speed that a plasma heat transport speed
    - Overall $\nabla_r T_i$ profile is "stiff", with the core $\nabla_r T_i$ responding to the edge plasma within only several milliseconds, while the plasma heat transport time scale is 10^2 slower.
- ITER operation assumes this experimental findings, but an agreeable physics understanding does not exist.
- Whole-volume first-principles modeling of background and turbulence dynamics → HPC is needed.

XGC1 gyrokinetic PIC code
(typically on 30K-220K cores, 1-10 wall-clock days)

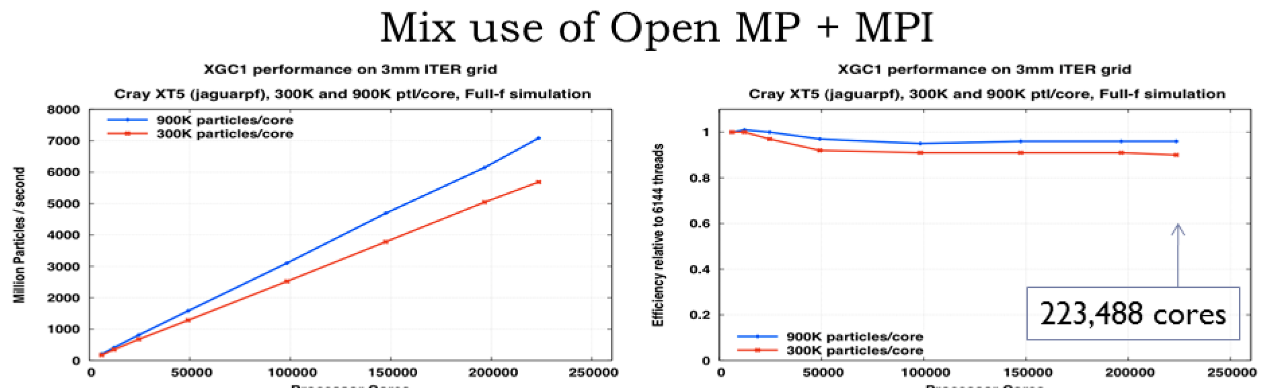
- **XGC1: full-f, X-point included Gyrokinetic Code in realistic tokamak geometry across magnetic separatrix surface**



- **Spatial simulation domain:** whole tokamak plasma volume with realistic tokamak edge geometry and Dirichlet wall boundary condition (grounded wall).
- **Unstructured triangular grid. Particles advance in cylindrical coordinate. Field solver on B-following grid.**
- **Capability in hand:** Electrostatic turbulence without scale-separation from mean plasma (ion) dynamics, with heat source and conserving Coulomb collisions
  - full-f ions and full-f electrons (for axisymmetric solution)
  - full-f ions and adiabatic electrons (for turbulent solution)
  - delta-f ions (for verification against other delta-f simulations)
- **Capability under development**: **Full-f electromagnetic turbulence**
  - Current capability: delta-f

XGC1 Scales efficiently on JaguarPF

Mix use of Open MP + MPI

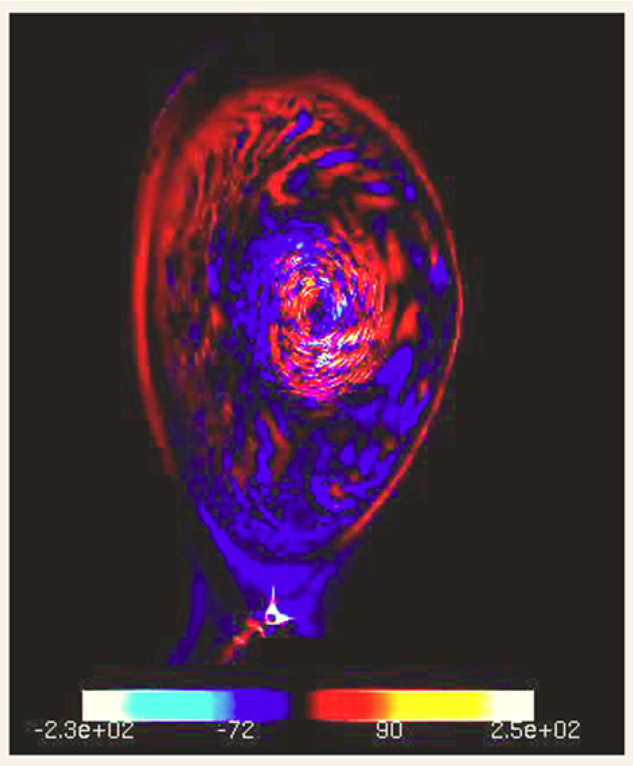


- **900K particles per thread problem is more computationally intensive than 300K problem, which leads to a somewhat higher particle push rate (by approx. 20%).**
- **Performance scaling is excellent for both problems.**

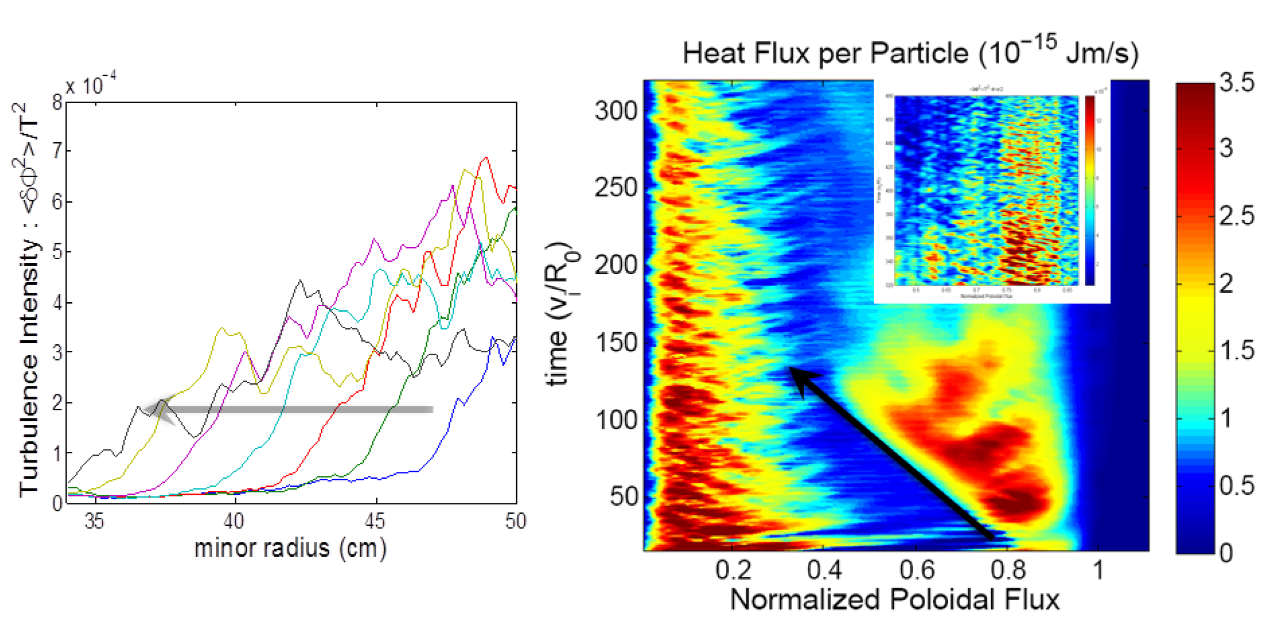
Jaguar PF (224K cores)	Average Job size	Utilization (core hours)
Jobs requesting <20%	3,079	8,446,978
Job requesting between 20% - 60%	66,474	3,042,575
Jobs requesting >60%	170,304	14,311,232

Whole-Volume, full-f ITG Simulation for DIII-D

- ITG (Ion Temperature Gradient) driven turbulence is the most robust and fundamental micro-turbulence in a tokamak plasma.
- Includes diverted edge geometry and magnetic axis
- Realistic Dirichlet BD condition $\Phi=0$ on conducting wall.
- Heat source in the central core
- This type of simulation is possible only on extreme HPCs → will push the edge of future HPC
- Several new scientific discoveries have emerged.



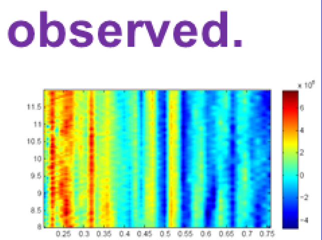
Edge turbulence propagates deep into the core and self-organizes the global temperature profile to criticality (SOC).

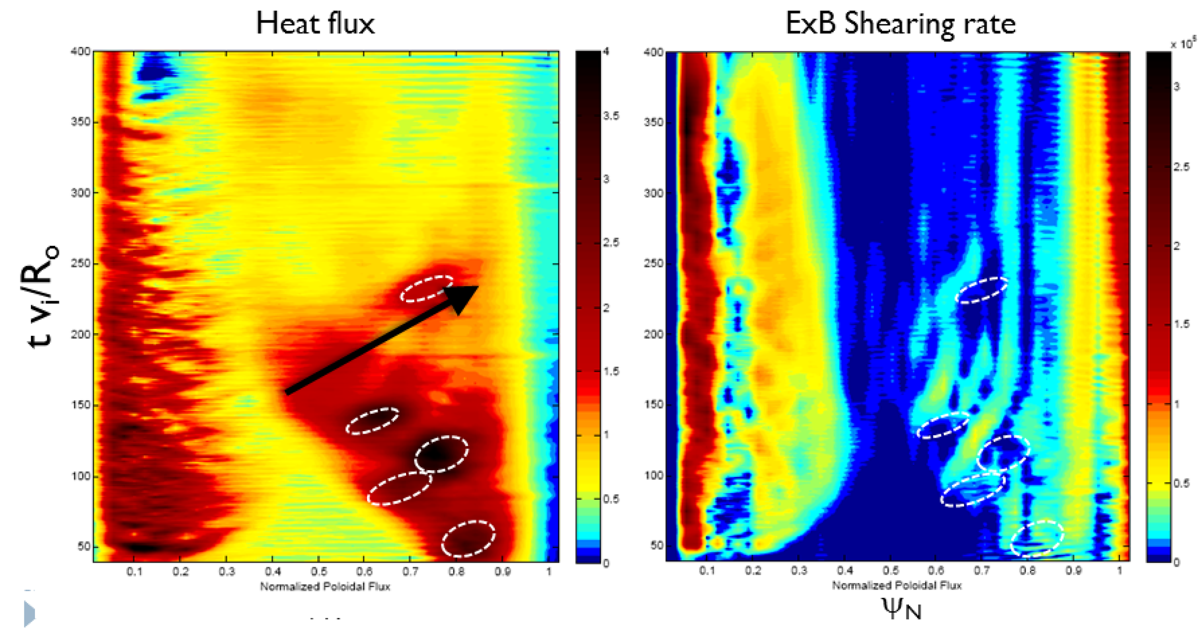


As edge turbulence arrives, local turbulence is aroused/modified and induces adequate heat flux to yield self-organized criticality.

Textbook type of turbulence interaction with self-organized ExB shearing dynamics is observed.

Turbulence propagation and heat burst settles down to quasi-steady SOC (avalanching) state in ~3-5 ms
→ Experimental core-edge interaction time.

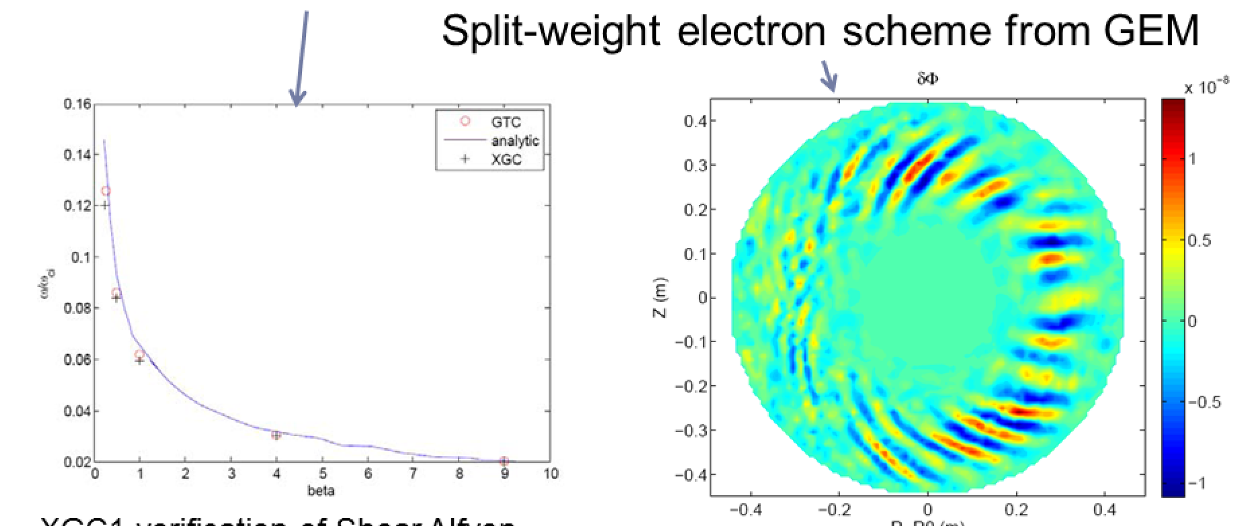




Moving Forward, riding on more extreme scale HPC: Electromagnetic turbulence in the whole volume

Fluid-kinetic hybrid electron scheme imported from GTC

Split-weight electron scheme from GEM



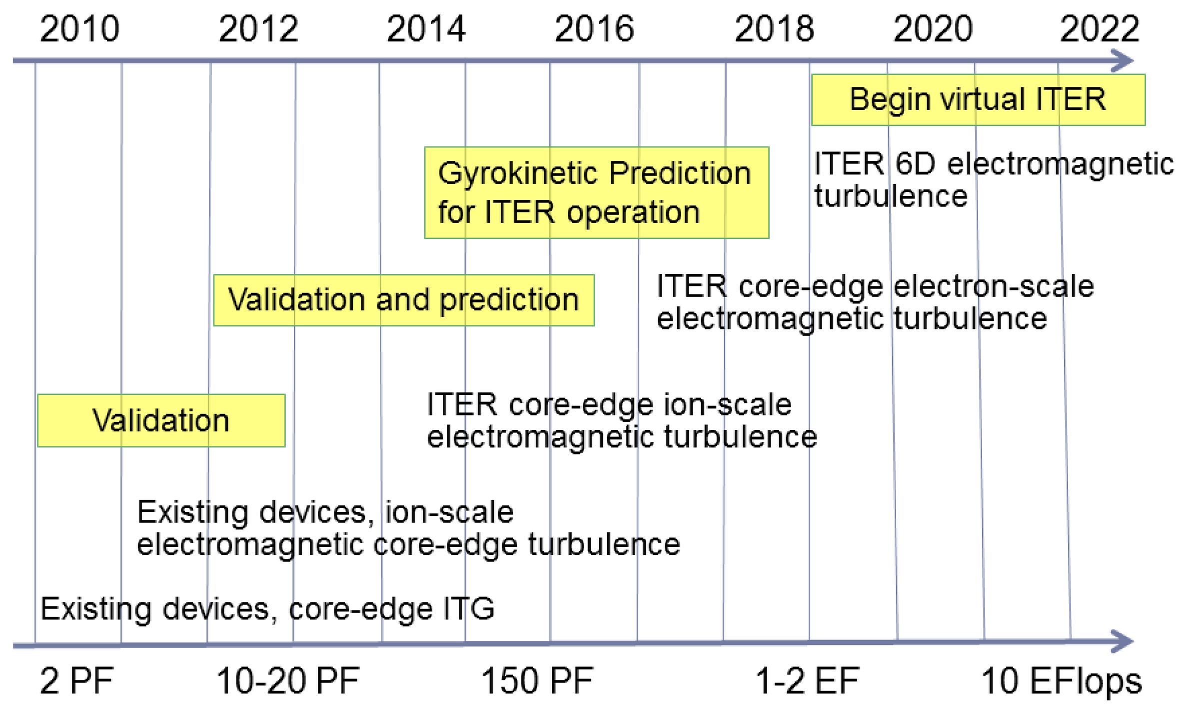
XGC1 verification of Shear Alfven wave. The line is from an analytic calculation, the "o" data points are from GTC and the "+" data points are from XGC1.

Split-weight-electron simulation of electromagnetic turbulence in XGC1 at low electron beta.

Looking forward to exascale simulation

- Examination of Hybrid, GPGPU, OpenMP, MPI programming.
- Advanced I/O pipelines for reduction of data movement in I/O.
- Memory localization with multi-domain decomposition with nearest-neighbor communication.
- Lack of computing power has been forcing us to study the 6D Vlasov plasma system in the reduced 5D system, restricting the kinetic simulation validity to << gyrofrequency and ≥ gyroradius.
- On exa-scale HPC, the dream of a 6D whole-volume tokamak simulation can be realized, but highly challenging: requires close co-design with computer science and applied mathematics.
  - Implicit time-marching to avoid CFL trouble with Alfven waves
  - How well can we localize the computation?
  - Efficient in-memory data staging and data analysis
  - Resiliency and fault tolerance?
  - Concurrency issue: dynamics load balancing?
  - How much can we improve I/O?
  - Flexibility to unknown new hardware and programming models

XGC1 Roadmap to Exascale (1 day run-target)



Conclusion

- XGC1 is a new generation fusion particle code, efficiently scaling to the maximal number of Jaguarpf cores.
  - Unlike other existing gyrokinetic codes, XGC1 simulates the whole-volume tokamak in realistic diverted magnetic field geometry in full-function (as opposed to the perturbative delta-f).
  - XGC1 performs multiscale background and turbulence dynamics in a single framework.
  - XGC1 has already made several scientific discoveries
- For a higher degree first-principles multiscale tokamak modeling in XGC1, more extreme scale HPC is needed.
  - XGC1 is getting ready for next generation HPC with the state-of-the-art computational and applied math technologies.
- If an exascale HPC is available in the future, fusion particle code can make a quantum jump into the formidable 6D tokamak physics simulation. An efficient co-design is a necessity.