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Simulation of negative triangularity plasmas with the GENE-X code

MANET project report, IFERC-CSC Workshop

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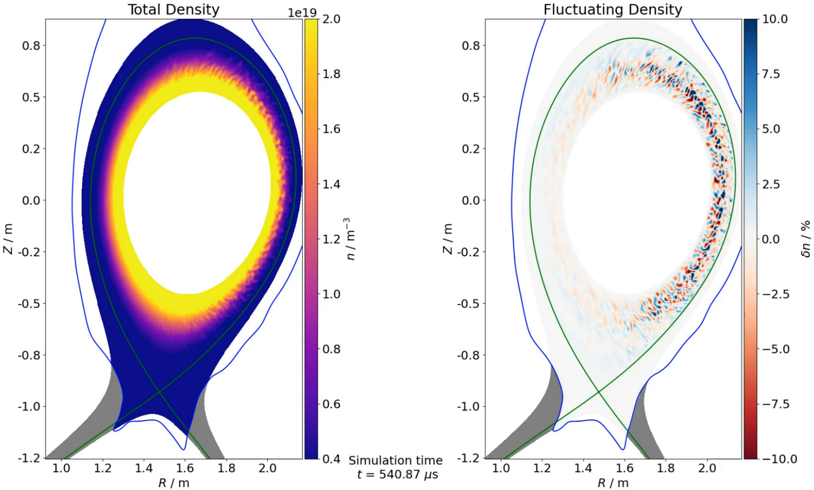
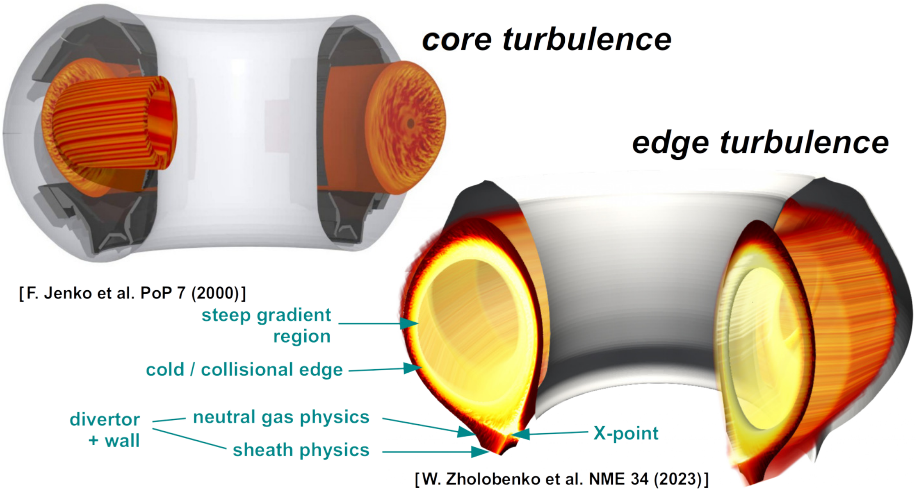
This work was carried out using the JFRS-1 supercomputer system at Computational Simulation Centre of International Fusion Energy Research Centre (IFERC-CSC) in Rokkasho Fusion Institute of QST (Aomori, Japan).

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

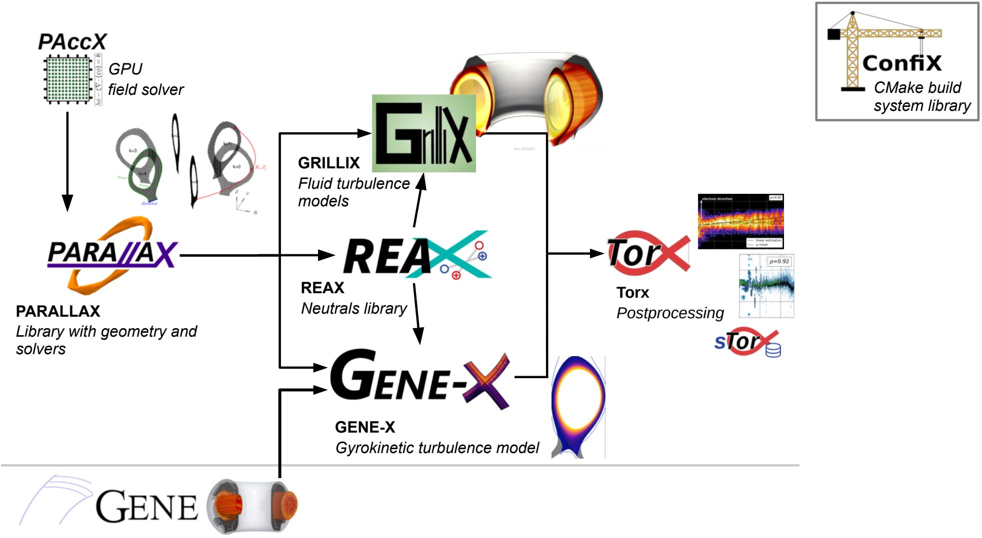
GENE-X simulates global gyrokinetic turbulence in the edge and scrape-off-layer (SOL) of X-point geometries



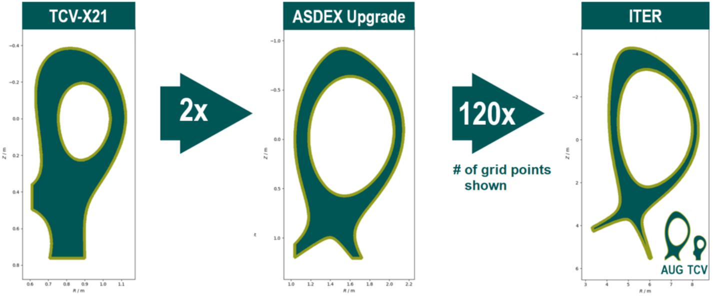
Simulating edge and SOL turbulence is a challenging task



Our group developed a unique edge turbulence code framework



Our goal is towards first-principles predicitive simulations in reactor-sized machines



Today's standard application:
medium-sized tokamaks

Target goal:
reactor-sized machines

Simulation challenges:

- Performance
- Physics accuracy
  $\rightarrow$ validation study required

EUROFusion roadmap:

- Good confinement avoiding ELMs
  $\rightarrow$ example: negative triangularity (NT)
- Heat exhaust

In this talk we present results obtained with JFRS-1 supercomputer

Part I

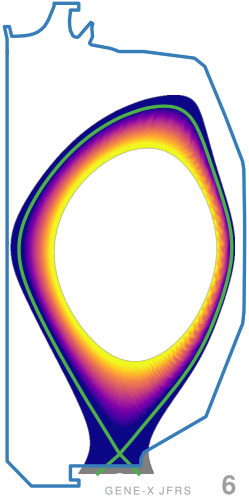
- Overview of the GENE-X code

Part II

- Validation of GENE-X in negative triangularity DIII-D

Part III

- Overview of other studies (analysis ongoing)

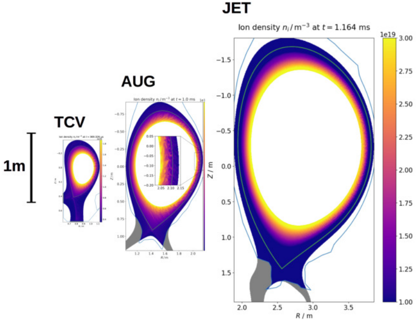


GENE-X code overview

GENE-X enables gyrokinetic turbulence simulations in X-point geometries

Features:

- grid-based (Eulerian)
- global
- non-linear
- full-f
- electromagnetic (EM)
- collisional



GENE-X can simulate from the core to the wall.

Efficiently designed for massively parallelized CPU-based supercomputers. Strong scaling with >90% efficiency up to 2048 nodes (≈ 100k cores).

[D. Michels, A. Stegmeir, P. Ulbl et al. CPC 264 (2021)] [D. Michels, P. Ulbl et al. PoP 29 (2022)] [P. Ulbl, T. Body et al. PoP 30 (2023)]

GENE-X solves a full-f, collisional, EM gyrokinetic model

evolution | $\mathbf{B}^*$ advection | perpendicular drifts

$$\frac{\partial f_\alpha}{\partial t} + v_{||}\frac{\mathbf{B}^*}{B^*_{||}}\cdot\nabla f_\alpha + \frac{c}{q_\alpha B^*_{||}}\mathbf{b}\times\left(\mu\nabla B + q_\alpha\nabla\phi_1 + \nabla H_2\right)\cdot\nabla f_\alpha$$

$$-\frac{\mathbf{B}^*}{m_\alpha B^*_{||}}\cdot\left(\mu\nabla B + q_\alpha\nabla\phi_1 + \nabla H_2\right)\frac{\partial f_\alpha}{\partial v_{||}} - \frac{q_\alpha}{m_\alpha c}\frac{\partial A_{1,||}}{\partial t}\frac{\partial f_\alpha}{\partial v_{||}} = \sum_\beta C_{\alpha\beta}(f_\alpha, f_\beta)$$

vspace-advection | magnetic induction | collisions

with

$$-\nabla\cdot\left(\sum_\alpha \frac{m_\alpha c^2 n_\alpha}{B^2}\nabla_\perp\phi_1\right) = \sum_\alpha q_\alpha \int f_\alpha\,\mathrm{d}W, \quad -\Delta_\perp A_{1,||} = 4\pi\sum_\alpha\frac{q_\alpha}{c}\int v_{||} f_\alpha\,\mathrm{d}W.$$

$$\mathbf{B}^* = \mathbf{B} + \frac{m_\alpha c}{q_\alpha}v_{||}\nabla\times\mathbf{b} + \nabla A_{1,||}\times\mathbf{b}, \quad H_2 = -\frac{m_\alpha c^2}{2B^2}\left|\nabla_\perp\phi_1\right|^2, \quad \mathrm{d}W = 2\pi B^*_{||}/m_\alpha \mathrm{d}v_{||}\mathrm{d}\mu.$$

Based on [D. Michels, P. Ulbl, W. Zholobenko et al., PoP 29 (2022) 032307].

Collision models of varying fidelity are available in GENE-X

Bhatnagar-Gross-Krook (BGK)

$$C_{\alpha\beta} = \nu_{\alpha\beta}\left(\frac{B}{B^*_{||}}\mathcal{M}_{\alpha\beta} - f_\alpha\right).$$

Lenard-Bernstein/Dougherty (LBD)

$$C_{\alpha\beta} = \frac{\nu_{\alpha\beta}}{B^*_{||}}\left\{\frac{\partial}{\partial v_{||}}\left[\left(v_{||} - u_{||,\alpha\beta}\right)B^*_{||}f_\alpha + \frac{1}{2}v^2_{\mathrm{th},\alpha\beta}\frac{\partial B^*_{||}f_\alpha}{\partial v_{||}}\right]\right.$$
$$\left. + \frac{\partial}{\partial\mu}\left[2\mu B^*_{||}f_\alpha + \frac{m_\alpha v^2_{\mathrm{th},\alpha\beta}}{B}\mu\frac{\partial B^*_{||}f_\alpha}{\partial\mu}\right]\right\}.$$

- Conservative finite volume discretization (2nd order)

Fokker-Planck/Landau (FPL)

$$C_{\alpha\beta} = -\frac{1}{B^*_{||}}\frac{\partial}{\partial\mathbf{v}}\cdot\left[B^*_{||}\left(\mathbf{E}_{\alpha\beta}f_\alpha + \mathbf{D}_{\alpha\beta}\cdot\frac{\partial}{\partial\mathbf{v}}f_\alpha\right)\right],$$
$$\mathbf{E}_{\alpha\beta} = \frac{\Gamma_{\alpha\beta}}{m_\beta}\int \mathrm{d}\mathbf{v}'\,\mathbf{U}^{\mathrm{E}}_{\alpha\beta}\cdot\frac{\partial}{\partial\mathbf{v}'}f'_\beta,$$
$$\mathbf{D}_{\alpha\beta} = -\frac{\Gamma_{\alpha\beta}}{m_\alpha}\int \mathrm{d}\mathbf{v}'\,\mathbf{U}^{\mathrm{D}}_{\alpha\beta}f'_\beta,$$
$$\mathbf{U}^{\mathrm{E}}_{\alpha\beta} = \begin{pmatrix} U_{\perp,\perp} & U_{\perp,||} \\ U_{||,\perp} & U_{||,||}\end{pmatrix},\quad \mathbf{U}^{\mathrm{D}}_{\alpha\beta} = \begin{pmatrix} U_{\perp,\perp} & U_{\perp,||} \\ U_{\perp,||} & U_{||,||}\end{pmatrix}.$$

- Components of **U** are given by linear combinations of elliptic integrals $E(m)$, $K(m)$
- 2nd order FV discretization

See [R. Hager et. al, JCP315 (2016)]

[P. Ulbl, D. Michels and F. Jenko, Contrib. Plasma Phys. 2021, e202100180]

Boundary conditions provide heat and particle fluxes in our simulations

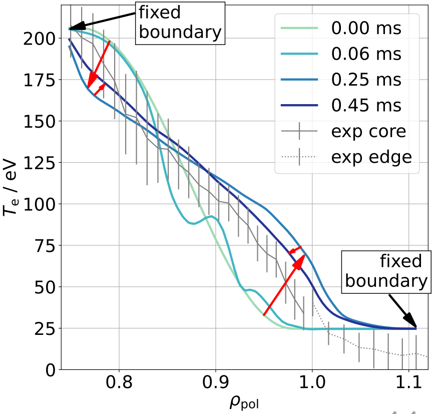
"First-principles" modelling: we start from an arbitrary initial state, not imposing the experimental profiles as a whole.

GENE-X BCs

Dirichlet with

- **Distribution function**: Maxwellian with experimental profile values for n and T (no flow)
- **Potentials**: zero

New: flux driven mode available



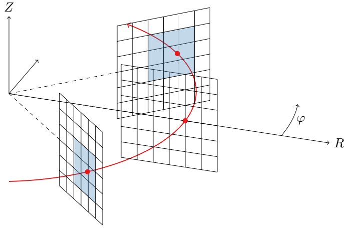
The Flux-Coordinate Independent Approach (FCI) allows for simulations in X-point geometries

Plasma turbulence is field aligned, **but** conventional field aligned coordinates break down at the X-point.

Solution: FCI approach

- Collection of Cartesian poloidal planes.
- Connected with magnetic field lines.

$\rightarrow$ **locally field aligned coordinates.**



Discretization:

$\perp$

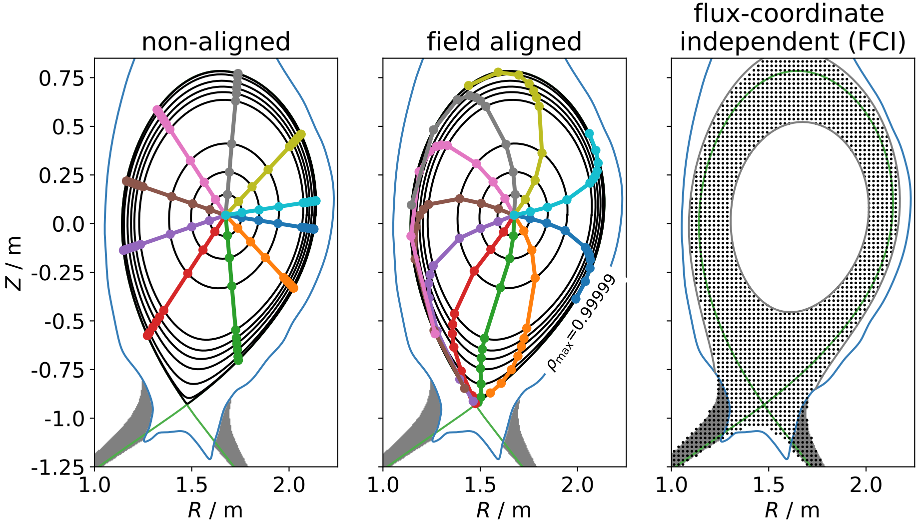
- 4th order sym. FD for $x, z, v_{||}$ derivatives
- 2nd order Arakawa for non-linear terms
- 2nd order elliptic solvers (GMRES + multigrid))

$||$

- Field line tracing
- Bicubic interpolation
- 4th order sym. FD for y

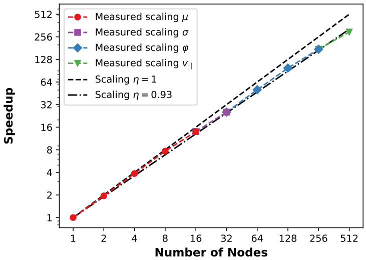
[D. Michels, A. Stegmeir, P. Ulbl et al., CPC 264 (2021) 107986]

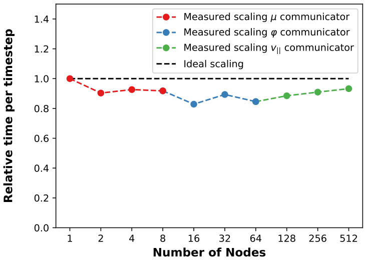
FCI vs. field-aligned



GENE-X utilized efficient hybrid MPI+OpenMP parallelization

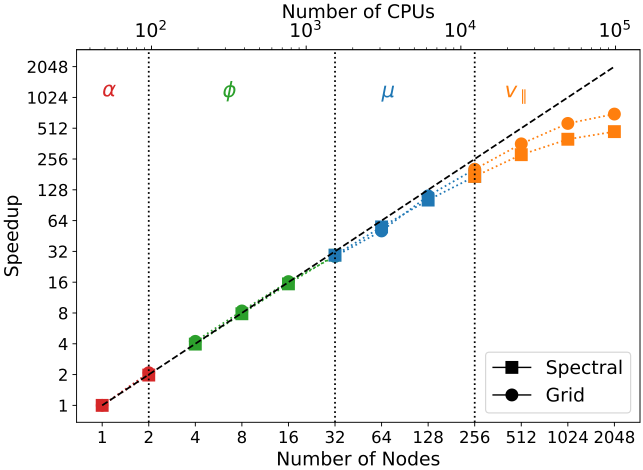
- Hybrid MPI+OMP. MPI in $\varphi, v_{||}, \mu, \alpha$. OMP in RZ
- Typical problem size approx. $(RZ, \varphi, v_{||}, \mu, \alpha)$ = $(200000, 32, 80, 20, 2)$
- Example: production runs on Raven supercomputer (MPCDF)
  320 nodes - 72 cores. 640 MPI procs, 36 cores for OMP.
  MPI decomposition e.g. $(RZ, \varphi, v_{||}, \mu, \alpha)$ = $(1, 16, 2, 10, 2)$.
- Good strong (left) + weak (right) scaling on MPCDF Cobra





[D. Michels, PhD Thesis, TU Munich (2021)]

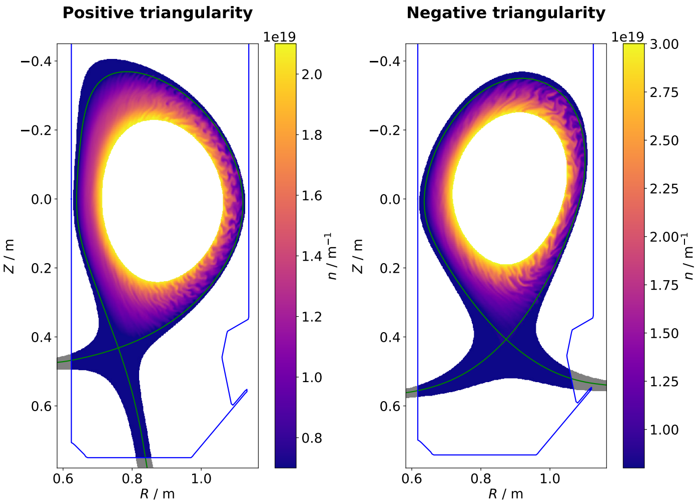
New strong scaling results on SuperMUC show excellent parallel efficiency on up to 100k cores



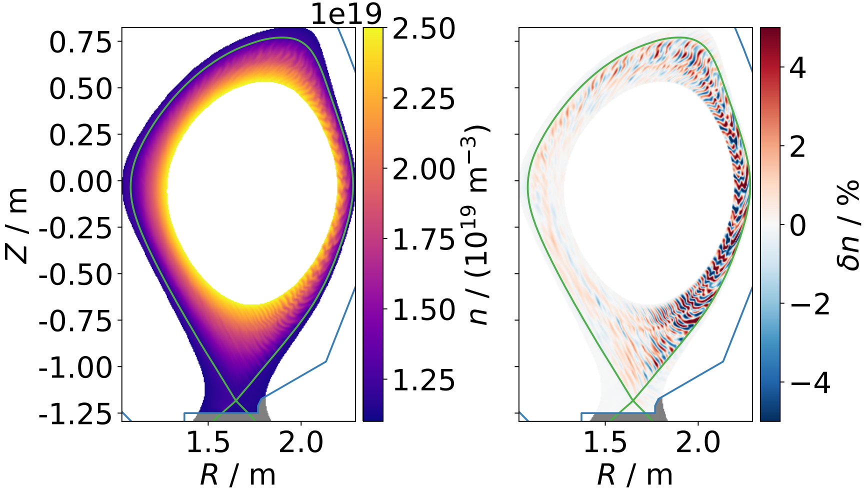
- Tested up to 2048 nodes with 48 cores each, around 98000 cores (4096 MPI procs, 1 per socket)
- As number of procs increases, communication starts to become a bottleneck
- Simulations are performed on >1k nodes on this machine
- Thanks to B. Frei for performing this analysis

Simulations performed on JFRS (analysis ongoing)

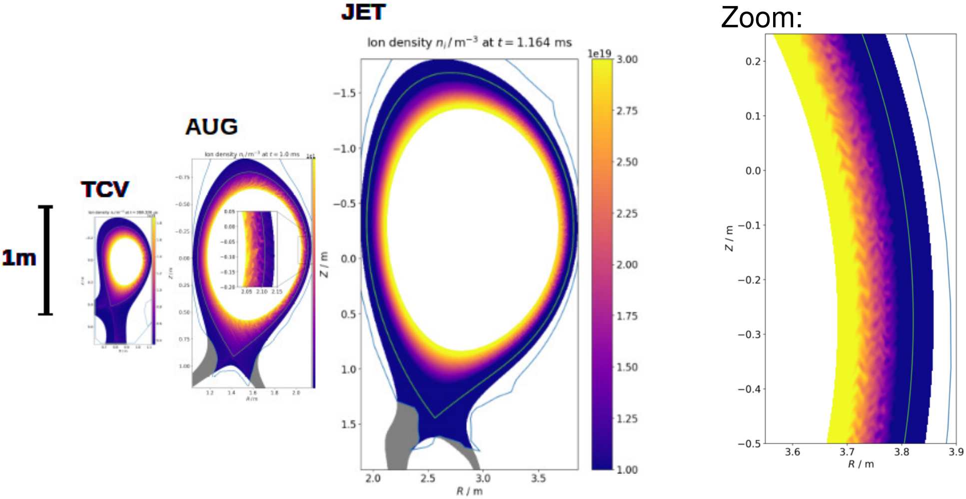
DTT-like shapes in NT/PT TCV were simulated to study geometry effects on turbulence



GENE-X was validated against diverted negative triangularity DIII-D scenario



First global gyrokinetic edge and SOL turbulence simulation in JET has been performed



Summary

- **GENE-X is able to perform first-principles turbulence simulations in X-point geometry (and stellarators now)**
- Hybrid MPI-OpenMP parallelization with >90% efficiency up to 100k nodes
- **First global grid-based GK turbulence simulations in DIII-D NT including the X-point** show **excellent agreement of profiles**. **Analysis ongoing.**
- Simulated pair of NT/PT discharges in TCV DTT-like shapes. **Analysis ongoing.**
- **First global gyrokinetic simulations of edge and SOL turbulence in JET**. Ti=Te approximation is supported. **Analysis ongoing.**
- **Performance and physics-wise, simulations of JT60-SA are now possible**

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