Demonstrator 1: Gysela-X++
Goal: Exascale plasma turbulence simulations

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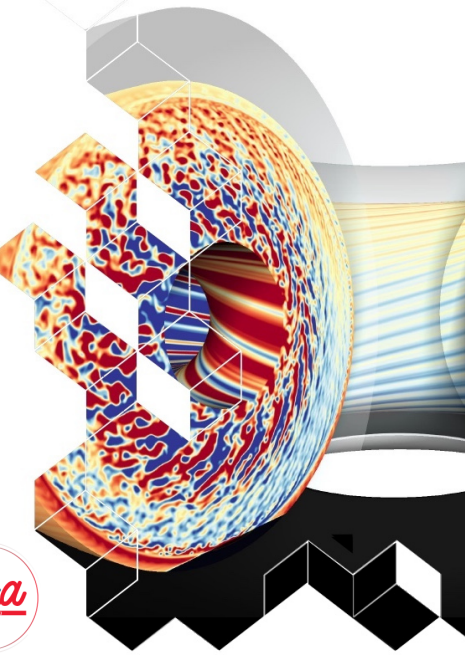

CExA Steering Commitee

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GYSELA code for exascale plasma turbulence simulations

- Gyrokinetic plasma turbulence simulations to understand turbulent transport that mainly governs confinement in Tokamaks
- GYSELA developed at IRFM/CEA code over 20 years thanks to strong EU collaboration between physicists, mathematicians and HPC specialists
  - MPI/OpenMP Fortran90 code optimized up to 730k CPU cores
  - Relative efficiency of 85% on more than 500k cores and 63% on 730k cores on CEA-HF (AMD EPYC 7763)
- Intensive use of petascale resources: $\sim$ 150 millions of hours / year (GENCI + PRACE + HPC Fusion resources)
- **Exascale needs for ITER plasma turbulence simulations**

Roadmap for GYSELA towards exascale simulations

Development of a new code Gysela-X++ ⇒ Why ?

- HPC challenge : **A portable code on new exascale architectures**
  - Heterogeneous accelerated nodes are extremely challenging

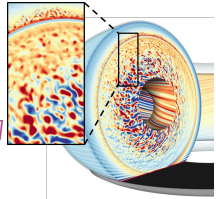
  → **modern C++ with** MPI + **Kokkos** *[E. Malaboeuf (CINES) 2024-2027]*
- **More physics** → new numerical challenges
  - **More realistic density & temperature gradients at edge-SOL**

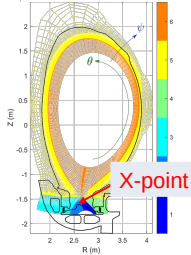
  → SL scheme for non-uniform meshes *[E. Bourne (CEA) 2020-2023]*
  - **X-point** geometry

  → SL scheme for multi-patches *[P. Vidal (IPP) PhD 2022-2025]*

  → 2D multi-patches poisson solver *[A. Hoffmann (IPP) 2023-2026]*
  - **Stellarator** configuration

  → 3D scalable Poisson solver *[S. Dasari (CERFACS) 2024-2027]*



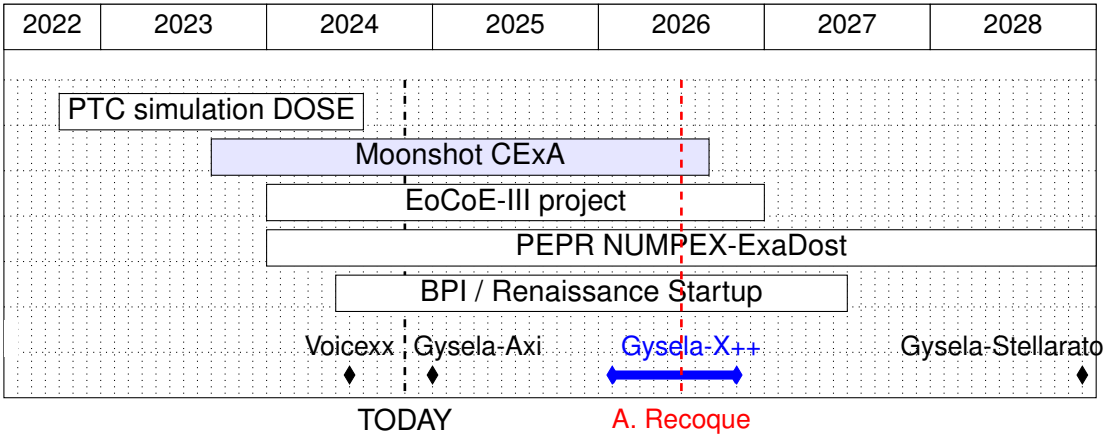


SOLEDGE-3X
X-point geometry

ITER schematic view

Roadmap for Gysela-X++ code towards exascale

First objective: Efficient parallel code to exploit Alice Recoque resources



A modular framework based on multiple libraries

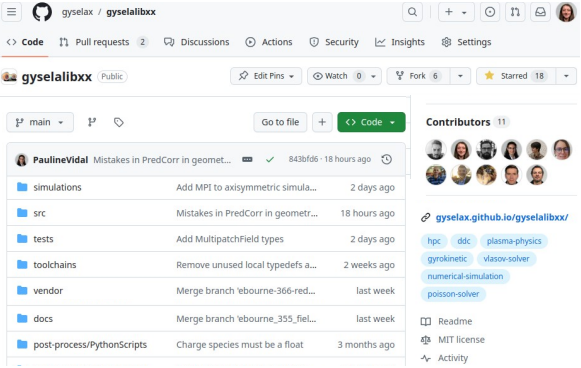
- **Modern C++ with MPI + Kokkos** based on external libraries:
  - DDC `https://github.com/CExA-project/ddc`: A discrete domain computation library to offer to the C++/MPI world an equivalent to the xarray.DataArray/dask. DDC relies on Kokkos and mdspan to offer CPU/GPU performance-portable multi-dimensional arrays and iterators.
  - Kokkos-kernels for FFT and Splines *[Y. Asahi et al., 2024]*
  - Gingko `https://ginkgo-project.github.io/` or eigen for Linear Algebra
  - libkoliop `https://gitlab.com/cines/code.gysela/libkoliop` for collision operator
  - PDI Data Interface `https://github.com/pdidev/pdi` for I/O
- Pros: Takes advantage of optimisation of each library on accelerated architectures
- Cons: Complex installation $\rightarrow$ Need for robust packaging tools (spack, GUIX, ...)

Gyselalibxx: A collection of C++ components

for writing gyrokinetic semi-lagrangian codes

- Computing kernels **ready for non-uniform meshes** + WIP for multi-patches.
  - Vlasov solver
    - Advection operators
    - Collision operators
    - Source terms
  - Poisson solvers
- **Vlasov-Poisson simulations**
  - 1X-1V Landau damping
  - 1X-1V Bump-on-Tail instability
  - 2X-2V Landau damping

`https://github.com/gyselax/gyselalibxx/`



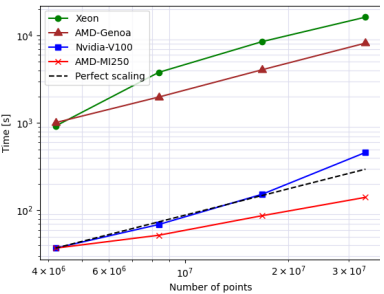
Packaging via spack or Guix + Doxygen doc.
+ CI integration (425 tests)

First prototype (2D mono-GPU): Voicexx code

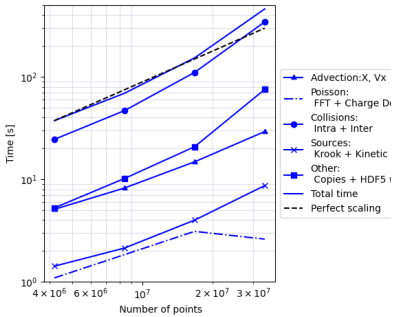
1X-1V semi-Lagrangian Vlasov code for sheath simulations

- See *[E. Bourne et al., 2023]* for numerics & *[Y. Munschy et al., 2023]* for physics
- **CExA demonstrator fully based on Kokkos**: Portable on multi-architectures

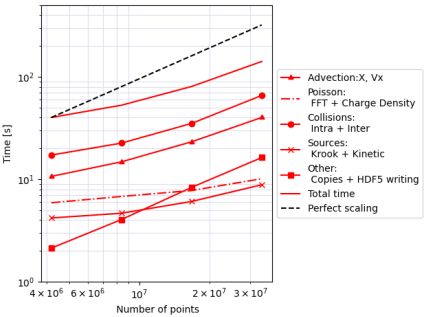
CPU versus GPU



GPU: NVIDIA V100



GPU: AMD-MI250X



- **Ready for physics**: neutrals *[PhD M. Perey]* **+ AI**: PINN's studies (NTU Singapore)

WIP: 4D multi-GPU prototype: Gysela-Axi code

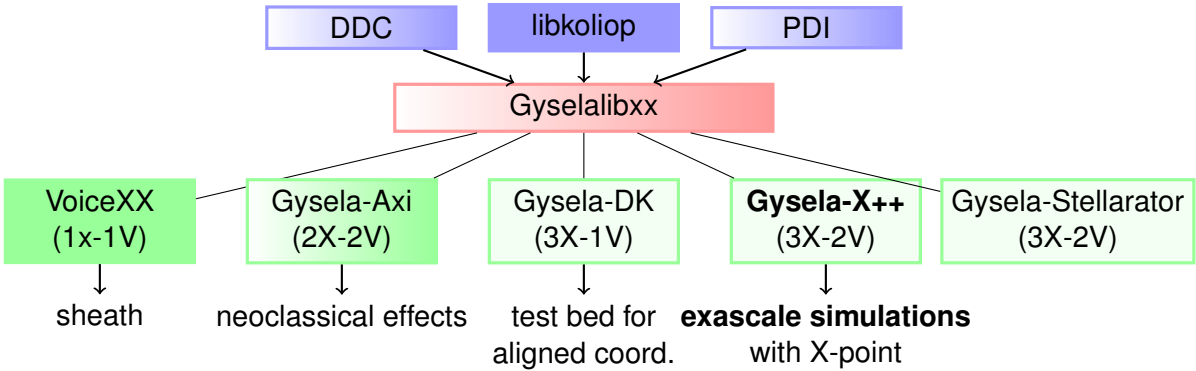
(2X-2V) semi-Lagrangian code for axisymmetric neoclassical simulations

- All the pieces of the puzzle are being put together
  - 2D advection in (r, θ) + 1D advection in $v_{\|}$
    - Non-uniform 1D and 2D splines **developed in DDC via PTC simu + optimized with kokkos-tools via Moonshot CExA**
  - 2D poisson solver in (r, θ)
  - 2D collision operator $(v_{\|}, \mu)$
    - translated from GYSELA F90 into C++ & Kokkos

    $\rightarrow$ libkoliop with an interface for both GYSELA F90 and Gysela-X++
  - MPI transposition
- Objective: end 2024 (EoCoE-III milestone)
  - Designed to work on multi-GPU optimization but also for physics:
    - Neoclassical effects with shaping and impurities *[PhD L. De Gianni]*

Conclusion & Perspectives (1/2)

- A **full based Kokkos ecosystem** under development **for gyrokinetic turbulence simulations** → Long time collab. with MdlS + Moonshot CExA clearly a booster
  → Exascale electromagnetic simulations for ITER plasma & stellarator



Conclusion & Perspectives (2/2)

Not possible without a strong collab. between HPC specialists, mathematicians and physicists

- Each prototype designed to be exploited by physicists
- **Future work with CExA team** (non-exaustive list):
  1. **Optimized 6D transposition** (3X-2V-species)
  2. **Optimised 3D and 4D splines**
  3. Training for new developers and for users
  4. Improvement of the readability
  5. Continuous Integration on multi-machines
- Missing numeric kernels for Gysela-X++ with X-point:
  - gyroaverage (will be extracted from GYSELA F90)
  - Vlasov + Poisson on multi-patches

Aknowledgments

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- IPP Garching - Germany: A. Hoffmann, P. Vidal, E. Sonnendrücker
- HLST CINES/Montpellier - France: E. Malaboeuf

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