# How to prepare the GYSELA-X code to future exascale edge-core simulations

Virginie Grandgirard, Y Asahi, J Bigot, E Bourne, Guilhem Dif-Pradalier, P Donnel, X Garbet, Ph. Ghendrih, Yaman Güçlü, K Kormann, et al.

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**Virginie GRANDGIRARD**

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[4] *SPC - Théorie. EPFL. PPB 315, CH-1015 Lausanne, Switzerland.*

[5] *IPP, Boltzmannstraße 2, 85748 Garching, Germany.*

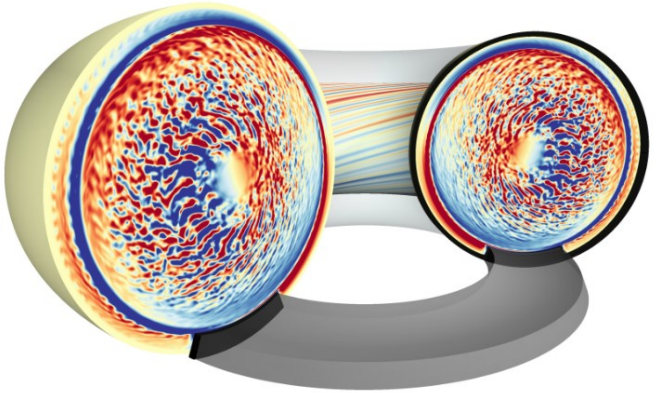
DE LA RECHERCHE À L'INDUSTRIE

# GYSELA-X = GYrokinetic SEmi LAgrangian code

- GYSELA-X a 5D gyrokinetic code based on a backward semi-Lagrangian scheme *[Grandgirard et al., CPC 2016]*

https://gyselax.github.io/

- GYSELA-X strength:
  - Global: simulate entire tokamak → boundary conditions (SOL-like, limiter)
  - Full-f: multi-scale physics
  - Flux-Driven (heat, momentum, … sources)
  - Multi-ion species → impurity transport
  - Multi-species collision operator → synergy neoclassical & turbulent transports
  - 3 electron modes : adiabatic (AE), full kinetic (FKE) or trapped kinetic electrons (TKE)
  - Electromagnetic effects (under validation)



HPC needs: 100 Mh/year

- GYSELA-X current physics interests:
  - Impact of magnetic configuration on turbulence *[post-doc: K. Obrejan 2020-2021] +*
  - → Adding of a more realistic geometry in GYSELA-X *[post-doc: P. Donnel sept 2021-2022]*
  - Core-edge turbulence: *[PhD: E. Bourne 2019-2022] +*
    - → How to numerically treat more realistic SOL *[PhD: Y. Munschy 2021-2024]*
  - Ripple *[PhD: R. Varennes 2019-2022]*
  - Impurity transport *[PhD: K. Lim 2019-2022]*

# Outline

- New numerical methods
  - Adding of more realistic geometry in the GYSELA-X code
  - Validation of semi-Lagrangian scheme with non-equidistant splines in VOICE (GYSELA mini-application)

- Improvement of the parallelisation
  - Optimisation of the collision operator
  - Optimisation of I/O : implementation of PDI in GYSELA-X

- Porting on new architecture for preparing to exascale simulations
  - First test on GPU with mini-applications (OpenACC/OpenMP or KOKKOS)
  - First feedback for GYSELA-X porting on ARM machines (FUGAKU/Japan + TGCC/France)

  → Do we need to rewrite GYSELA-X ? If yes, which choice ?

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# GYSELA-X improvement: Circular geometry replaced by a more realistic one

- **Culham equilibrium:** axisymmetric, second order accurate $O\left((r/R_0)^2\right)$ solution of the Grad-Shafranov equation

$$R = R_0 + \Delta(r) + \left(r - E(r) - P_{corr}(r)\right)\cos(\theta) + T(r)\cos(2\theta)$$
$$Z = \left(r + E(r) - P_{corr}(r)\right)\sin(\theta) - T(r)\sin(2\theta)$$

E → elongation, T → triangularity,
Δ:Shafranov shift, $P_{corr}$: flux surface relabelling

- SELALIB[1] Poisson solver recently coupled to GYSELA

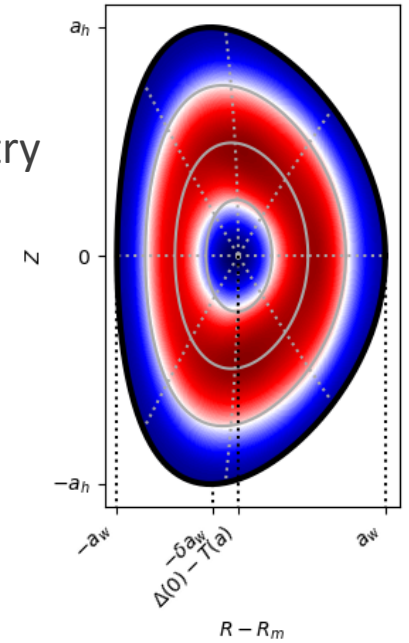
[1] *https://selalib.github.io/selalib/*

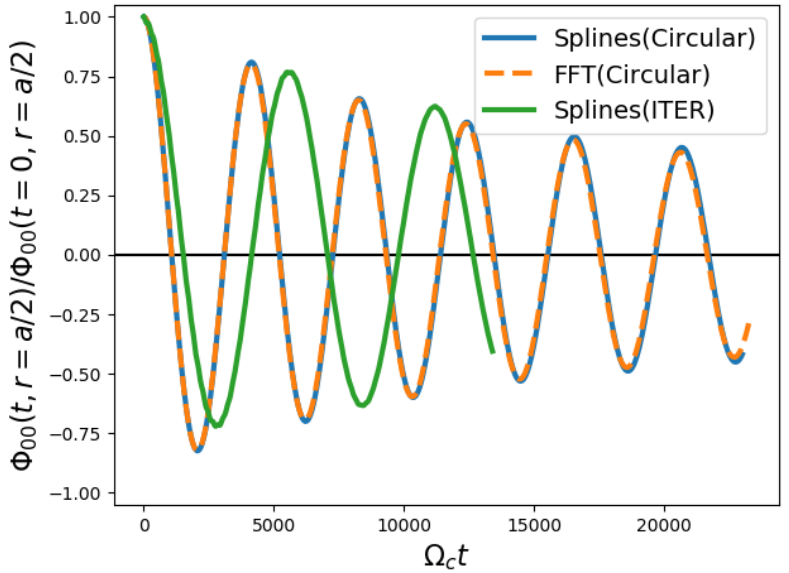
- First tests on GAM simulations with full-kinetic electrons for ITER-like geometry successfull

→ theoretical pulsation proportional to $\frac{1}{\sqrt{1+\kappa^2}}$ → ratio of 0.72 coherent with measured 0.74

ITER-like geometry
(κ=1.7, δ=0.4)

E(a)~=0.26*a
T(a)~=0.075*a




Good agreement in circular geometry between new solver (2D splines) and old one (finite difference in r and FFT in θ)

- 2D spline solver slower due to conjugate gradient iterations
→ Search of a better preconditionner still under investigation

*E. Bourne, K. Obrejan, X. Garbet, Ken Leleux + Y. Güçlü, K. Kormann (IPP Garching)*

# Limiter in GYSELA via immersed boundaries (penalisation technique)

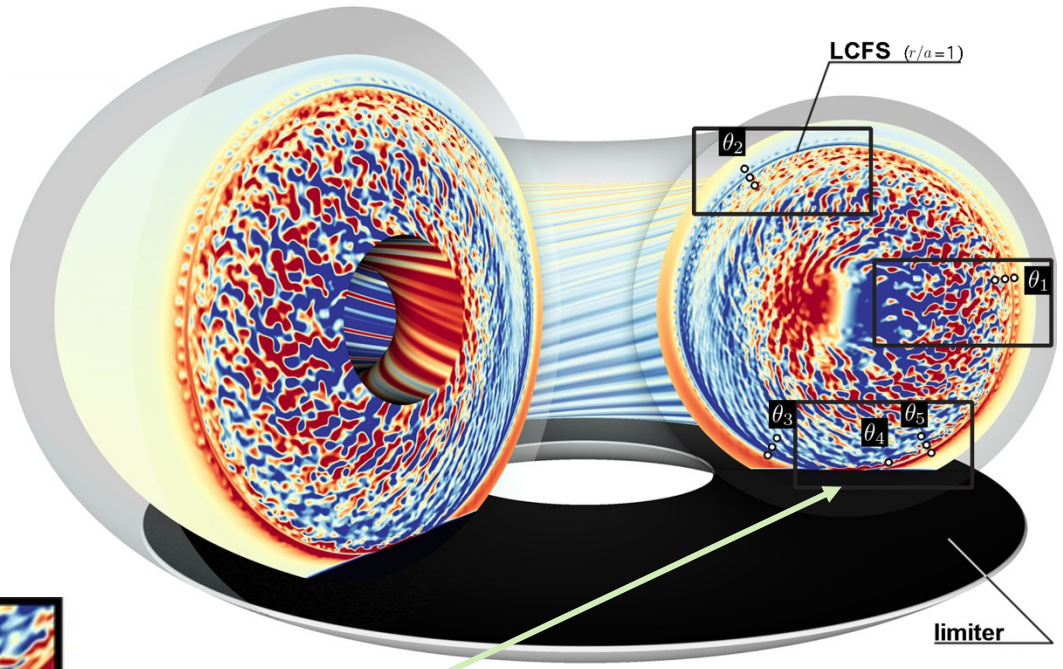
- **Flux-driven ITG turbulence** (adiab. electrons)
  $1/\rho^*=250$, $\nu^*=0.14$, global domain: $0 < \rho < 1.3$

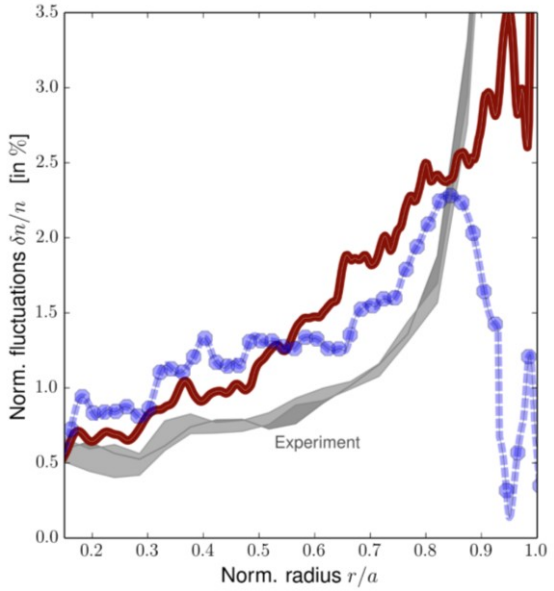
- PRACE 2020 simulation (TGCC/Irene ROME):

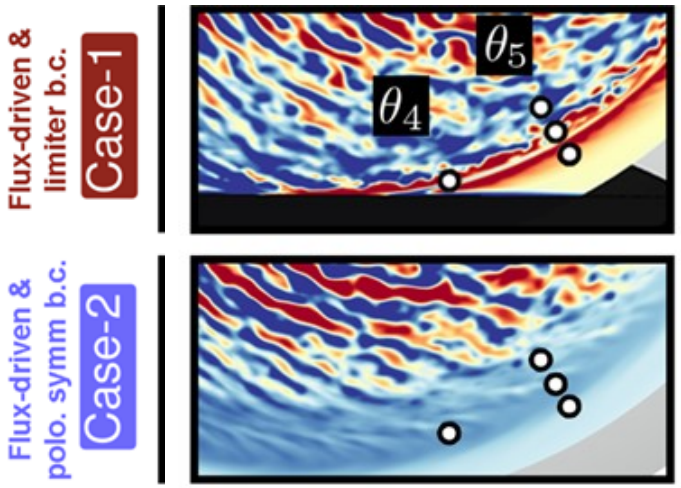
✓ 5D mesh ~ 100 billions of points
✓ ~ 6 millions of hours (~20 days on 12k cores)
✓ Several Tbytes of data

- Strong impact of boundary conditions on turbulence

*[Dif-Pradalier 2020]*



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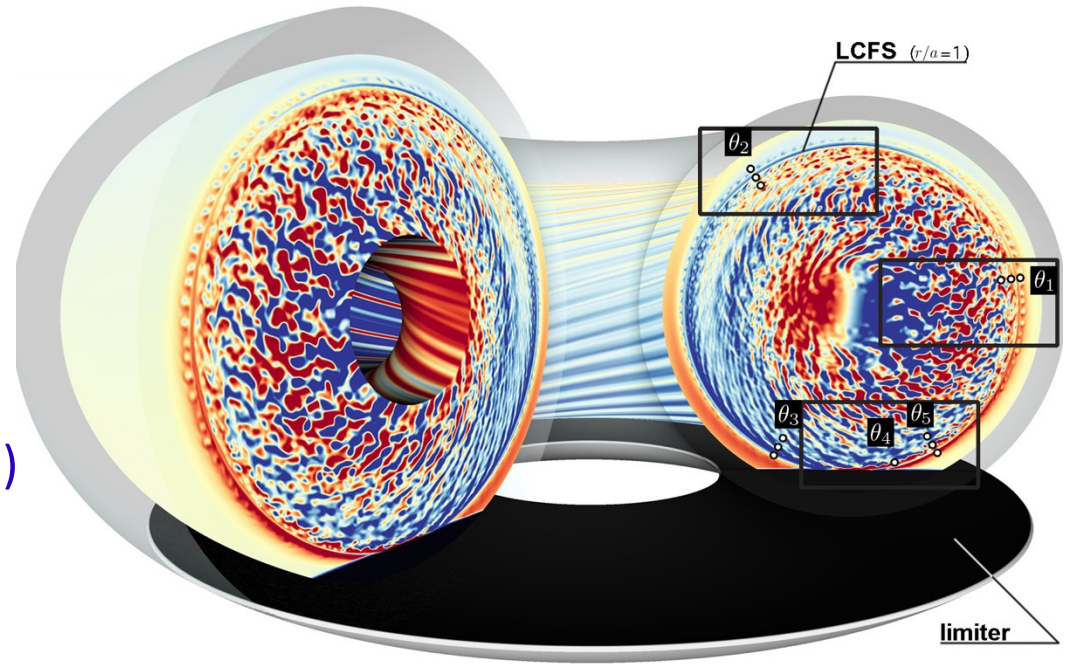
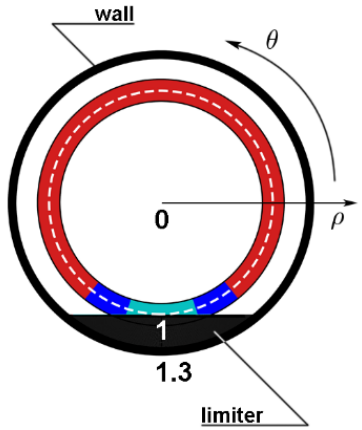
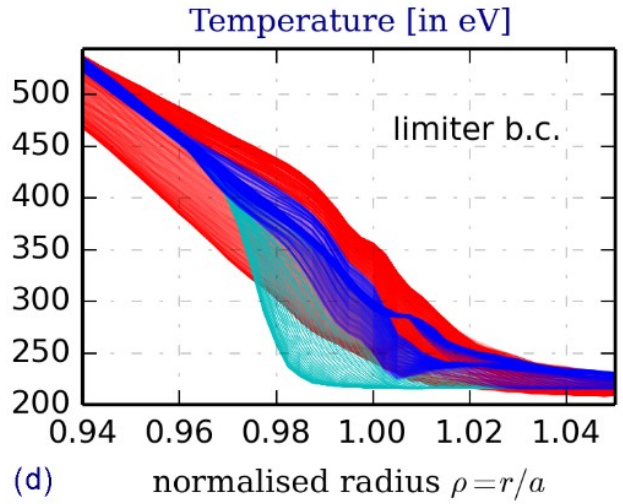
✓ 5D mesh ~ 100 billions of points
✓ ~ 6 millions of hours (~20 days on 12k cores)
✓ Several Toctets of data

- Strong density & temperature gradients close to the LCFS ($\forall\theta$)

*[Dif-Pradalier 2020]*




- How to treat more realistic temperature gradients ? (2 order of magnitude) → non-equidistant mesh

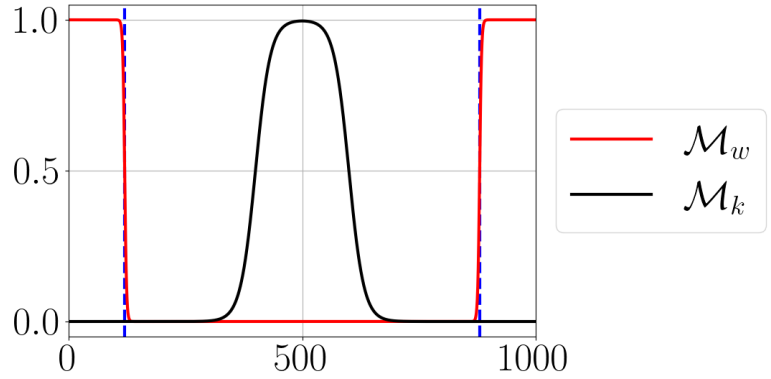
# VOICE – GYSELA mini-app to simulate sheath physics

- Solves normalised 1D-1D Vlasov-Poisson equation for particles of species s, mass $m_s$

$$\frac{\partial f_s}{\partial t} + \sqrt{\frac{m_e}{m_s}}\left(v_s \partial_x f_s + q_s(E_{ext} - \partial_x \phi)\partial_{v_s} f_s\right) = \nu_w \mathcal{M}_w (f_s - g_w) + \mathcal{M}_k S_v(v_x)$$

$$\partial_x^2 \phi = \frac{e}{\epsilon_0}\,(n_i - n_e)$$

$\nu_w$ is a measure of the restoring force which is localised at the mask $\mathcal{M}_w$
$g_w$ is a Maxwell-Boltzmann distribution function



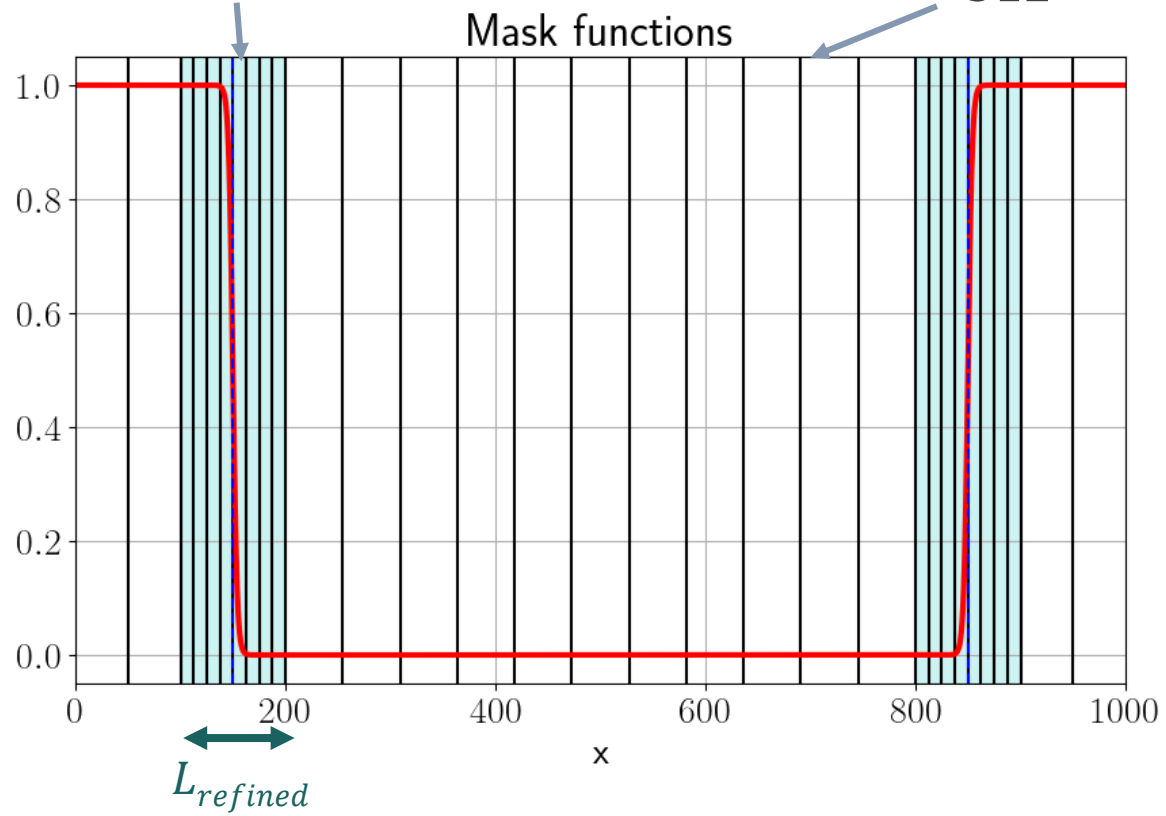

- Periodic in x, non-periodic in v
- Construct with GYSELA modules → Same numerical schemes
  - Backward semi-Lagrangian scheme (BSL)
    - 1D advection
    - Spline interpolation
  - Poisson solver (FEM or FD or FFT)
  - **Same penalization technique**

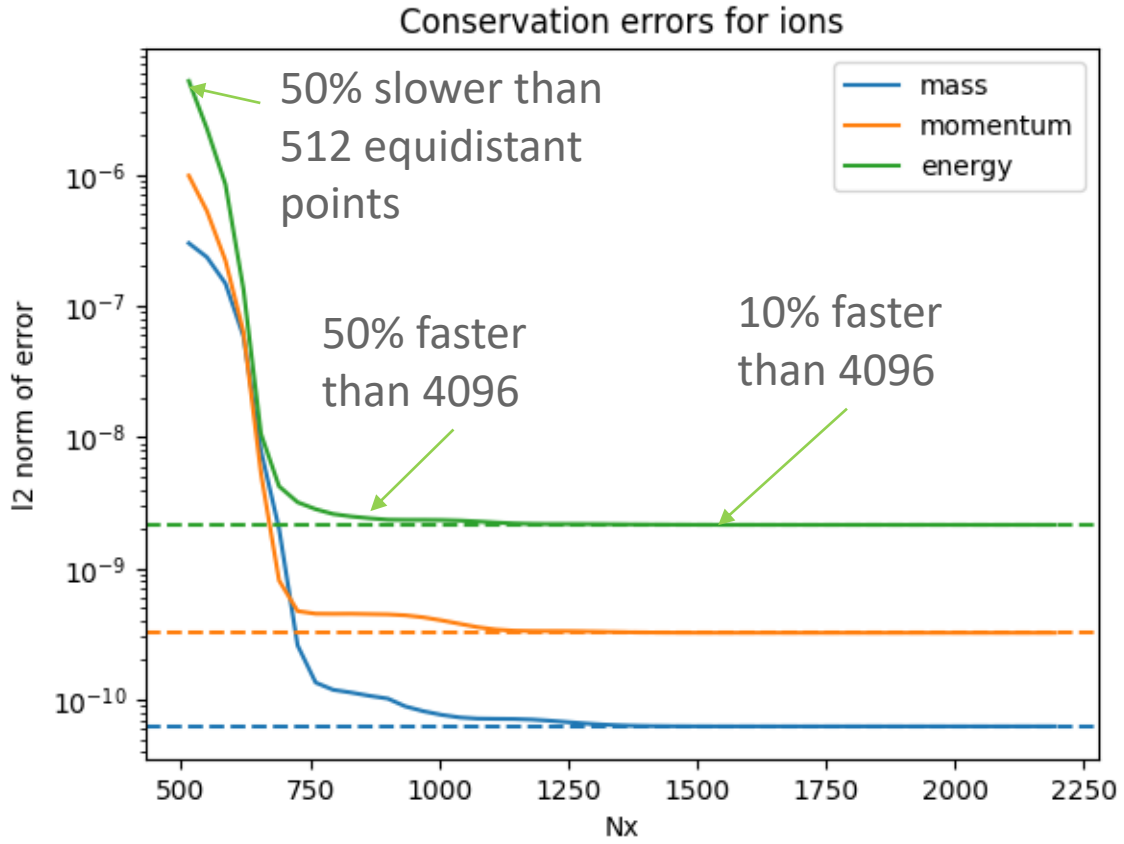
| VOICE | GYSELA |
|---|---|
| 2D (1D in x + 1D in v) | 5D (3D in x + 2D in v) |
| No parallelisation | MPI + OpenMP |
| Fortran + C++ | Fortran + few C modules |
| 10k lines | 50k lines |

- Testbed for BSL with non-equidistant splines before implementation in GYSELA-X code

# Non-equidistant splines to treat non-equidistant mesh → more accurate with less cost

$$dx_{refined} = \frac{Lx}{4096} \approx 0.25 \qquad dx = \frac{Lx}{512} \approx 2$$




$dx_{refined}$, $dx$ fixed and $0.5 < L_{refined} < 235$.

- Accuracy: same error with 1500 non-equidistant points and 4096 equidistant points.
- Non-equidistant points are slower as a binary search is needed to find the relevant basis spline and calculations cannot be simplified.

*E. Bourne, Y. Munschy, Ph. Ghendrih, G. Dif-Pradalier, Y. Sarazin + Y. Güçlü (IPP Garching)*

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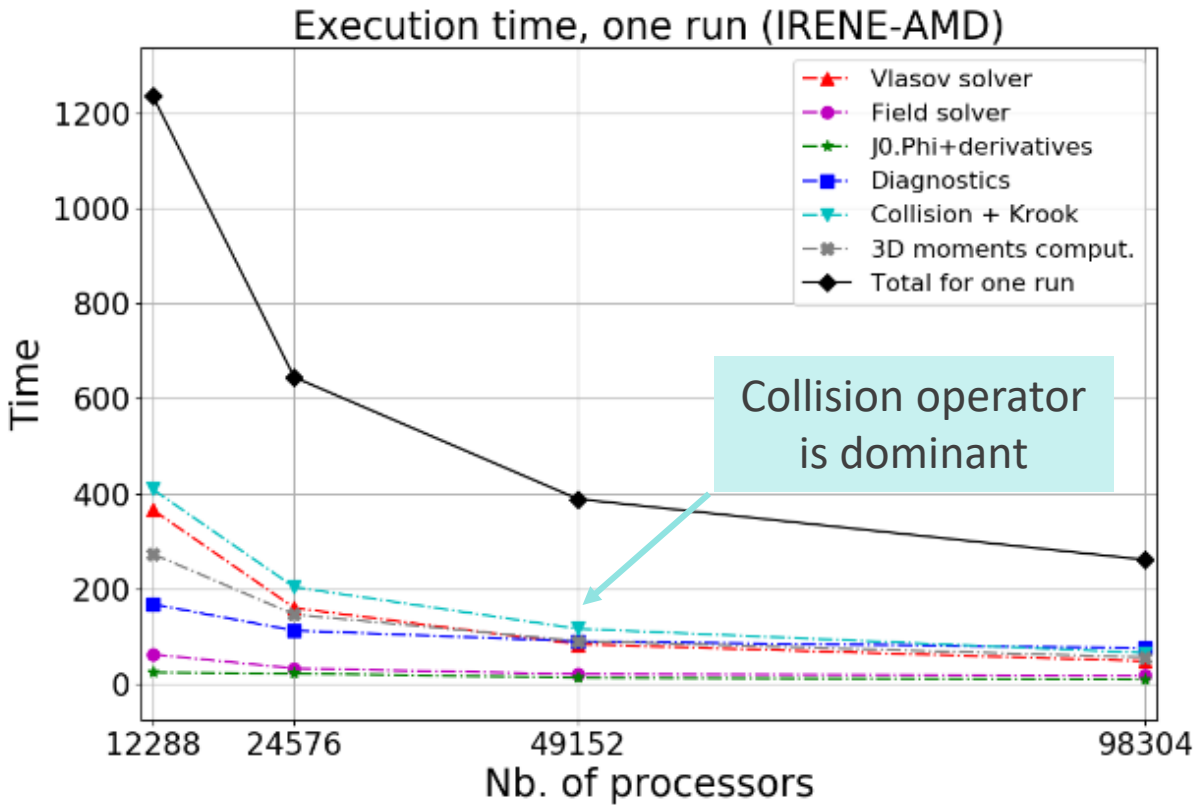
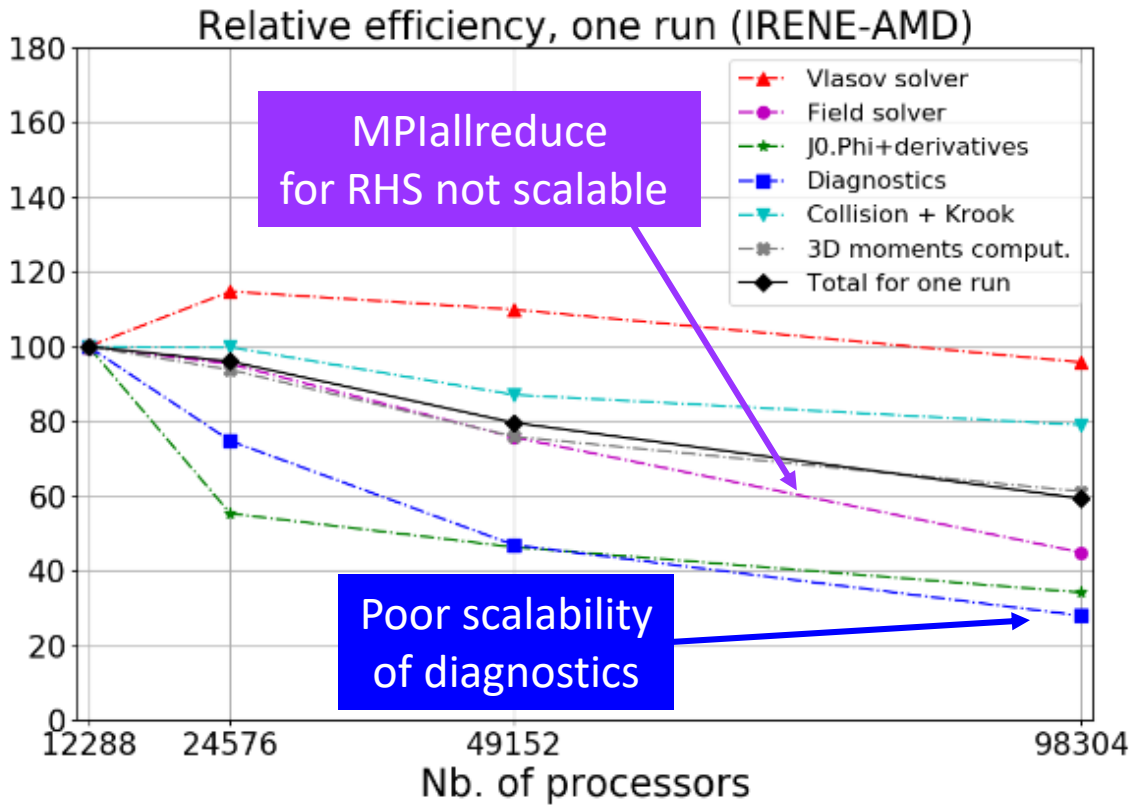
# GYSELA: Good scalability up to 100k cores

- GYSELA : MPI+OpenMP parallelism : 80% relative efficiency on 49,152 cores and 59% on 98,304 cores

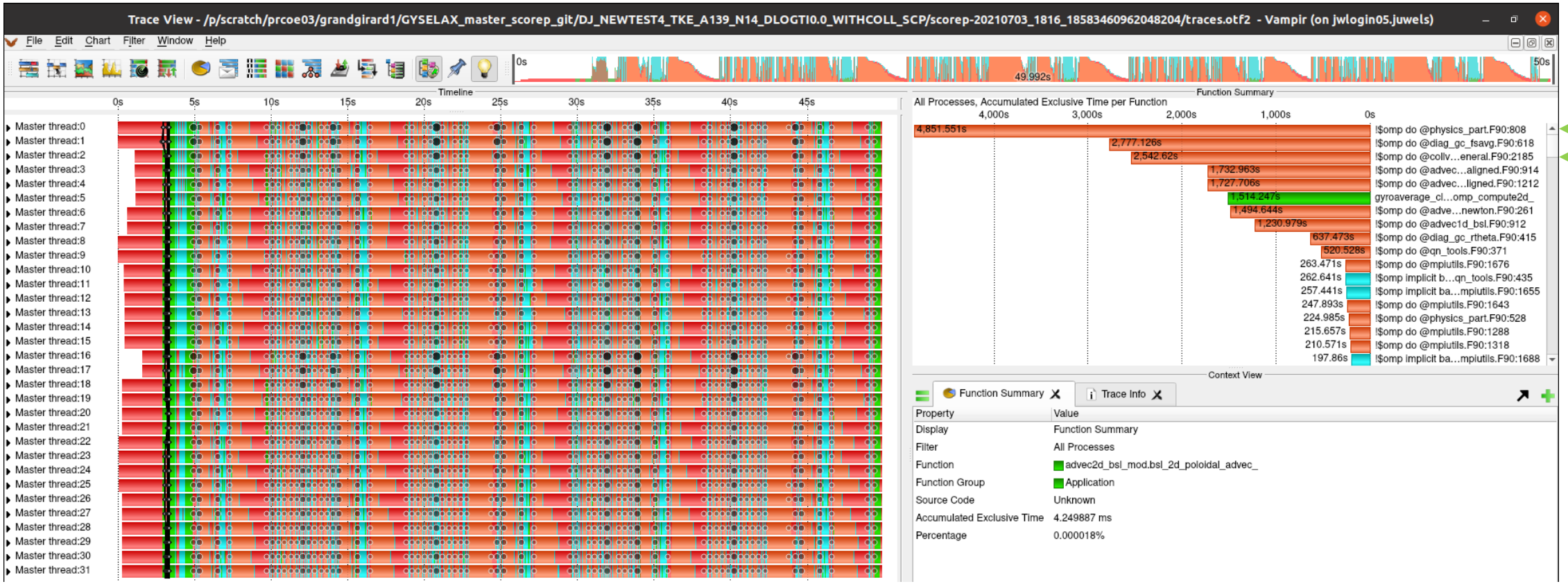



*« Strong scaling » of GYSELA code on Irene-AMD partition at TGCC-France (2020)*

- GYSELA : ~25% faster on IRENE-AMD than on IRENE-SKL. 2.3 times faster on IRENE-SKL than on IRENE-KNL

- Good load balancing due to eulerian nature of the semi-Lagrangian scheme (fixed grid in time)



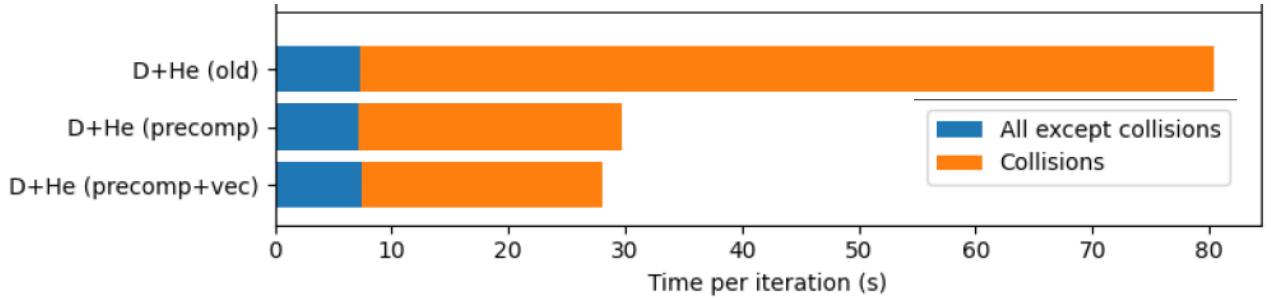

- Collision operator main drawback : Huge MPI communication to have all ($v_{//}$,$\mu$,all species) required data can't be avoided in the current MPI domain decomposition but can we improve the computation part ?
- Mid-term objective: Decouple diagnostics computation from computation kernels → First step: Use of PDI

# Multi-species collision operator extremely expensive

- With Score-p instrumentation on, in a simulation with one species, collisions ~50% of the total CPU time
  - Half of that taken by `I` and `J` (called several times on every point of the mesh at each time step)
  - Overall chain of functions `N_a_jl`→`L`→`I`→`J` very costly

| type | max_buf[B] | visits | time[s] | time[%] | time/visit[us] | region |
|---|---|---|---|---|---|---|
| ALL | 6,007,893,628 | 7,267,677,628 | 11237.66 | 100.0 | 1.55 | ALL |
| USR | 6,003,057,320 | 7,262,723,069 | 7375.43 | 65.6 | 1.02 | USR |
| OMP | 4,596,680 | 4,840,064 | 2830.14 | 25.2 | 584.73 | OMP |
| MPI | 413,576 | 73,197 | 1001.25 | 8.9 | 13678.85 | MPI |
| COM | 33,956 | 41,298 | 30.84 | 0.3 | 746.75 | COM |
| USR | 449,839,104 | 553,648,128 | 1009.56 | 9.0 | 1.82 | collvparmu_general_class.collvparmu_general_j_ |
| USR | 449,839,104 | 553,648,128 | 1688.50 | 15.0 | 3.05 | collvparmu_general_class.collvparmu_general_i_ |
| USR | 436,208,500 | 528,483,392 | 164.61 | 1.5 | 0.31 | utils_mod.utl_is_zero_ |
| USR | 436,207,746 | 528,482,464 | 367.15 | 3.3 | 0.69 | utils_mod.utl_locate_ |
| ● | ● | ● | ● | | | |
| USR | 224,919,552 | 276,824,064 | 277.10 | 2.5 | 1.00 | collvparmu_general_class.collvparmu_general_n_a_jl_ |
| USR | 224,919,552 | 276,824,064 | 524.05 | 4.7 | 1.89 | collvparmu_general_class.collvparmu_general_l_ |

- Rewritten of the innermost loop to add more vectorization




- CPU time gain of 1.9 (for 1 species) and 3.6 (for two species)

*K. Obrejan, P. Donnel (SPC/Lausanne)*

# PDI Data Interface for handling I/O as a data coupling → Towards in-situ diagnostics

https://pdi.julien-bigot.fr/master/

- PDI offers to exchange data between the application code and various external data handlers, such as for example the file-system for I/O or another code for code-coupling.
- New version of PDI recently implemented in GYSELA code
  - Instrumentation in the code via PDI_share, PDI_expose, PDI_reclaim

```
typedef enum { PDI_IN, PDI_OUT, PDI_INOUT } PDI_inout_t;

// A data buffer is ready (filled)
PDI_status_t PDI_share(const char *name, void *data, PDI_inout_t access);

// A buffer will be reused
PDI_status_t PDI_reclaim(const char *name);
```

  - Adding of a YAML configuration file for description of all the I/O data
  - HDF5 plugin choice used for diagnostics saving (~100 Gbytes)

```
plugins:
  decl_hdf5:
    - file: sp${pSpecies_id}/rprof_part_d${iter_diag:05d}.h5
      on_event: physics_part_save
```

  - Restart files (several Tbytes) saved in HDF5 but can be saved in FTI or SionLib by just changing the plugin

- PDI is a simple C/C++ API also available for Fortran and Python

```
/** Initializes PDI */
PDI_status_t PDI_init(PC_tree_t yaml_conf);

/** Finalizes PDI */
PDI_status_t PDI_finalize();
```

```
#     -> for toroidal angular momentum conservation
#       - Ltor          : toroidal angular momentum
#       - Tpol_psi      : polarization term
#       - Gamma_vE_r    : guiding-center turbulent flux
#                         (due to ExB velocity)
#       - Gamma_vEn0_r  : n=0 component of Gamma_vE_r
#       - Gamma_vD_r    : guiding-center neoclassical flux
#       - RSphi_vE_r    : toroidal Reynolds stress due to ExB
#       - RSphi_vEn0_r  : n=0 component of RSphi_vE_r
#       - RSphi_vD_r    : neoclassical toroidal Reynolds stress
LtorGC_FSavg:          { type: array, subtype: double, size: '$Nr+1' }
TpolGC_psi_FSavg:      { type: array, subtype: double, size: '$Nr+1' }
GammaGC_vE_r_FSavg:    { type: array, subtype: double, size: '$Nr+1' }
GammaGC_vEn0_r_FSavg:  { type: array, subtype: double, size: '$Nr+1' }
GammaGC_vD_r_FSavg:    { type: array, subtype: double, size: '$Nr+1' }
RSphiGC_vE_r_FSavg:    { type: array, subtype: double, size: '$Nr+1' }
RSphiGC_vEn0_r_FSavg:  { type: array, subtype: double, size: '$Nr+1' }
RSphiGC_vD_r_FSavg:    { type: array, subtype: double, size: '$Nr+1' }
```

- No extra cost for diagnostics as expected → First step before externalisation in Python
- Gain of a factor 10 for restart file writting still under investigation (temporary copy avoided + no checksum)
  - Big advantage: I/O optimization will be treated by specialists

*J. Bigot (MDlS-France) + Y. Ould-Ruis (INRIA-Grenoble/France)*

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# Porting VOICE on GPU → Is OpenACC a good candidate for GYSELA ?

- Participation to the IDRIS GPU Hackathon (4 days – May 2021).
- Objective: Accelerating VOICE via GPU parallelisation
  - Testing the complexity of the non-equidistant splines on GPU
- OpenACC parallelization of the splines + 1D advections + RHS → Gain factor of 5 to 8

**No parallelisation**

```
Elapsed time in advec x :     40.15840
Elapsed time in advec v :     82.60031
Elapsed time in RHS     :     33.78830
Elapsed time in Efield  :     8.750244
Elapsed time in diags   :     51.91985
Elapsed time in total   :     219.0524
```

**OpenACC parallelisation**

```
Elapsed time in advec x :     8.795156
Elapsed time in advec v :     10.38172
Elapsed time in RHS     :    0.5890590
Elapsed time in Efield  :     9.755074
Elapsed time in diags   :     56.86447
Elapsed time in total   :     90.60061
```

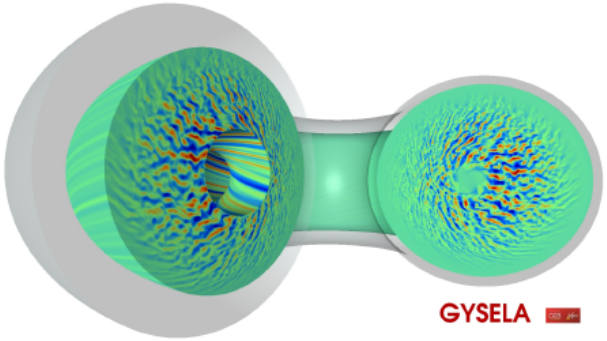
- First feedback : OpenACC parallelisation difficult due to presence of:
  - derived types + pointers + LAPACK routines (banded matrix)
- Not a big surprise: Requires lots of rewriting → This problem will be amplified for GYSELA
- GPU porting of GYSELA planned for the next two years

*E. Bourne, K. Obrejan, D. Midou + S. Touzet (IDRIS/France) + F. Spiga (NVIDIA)*

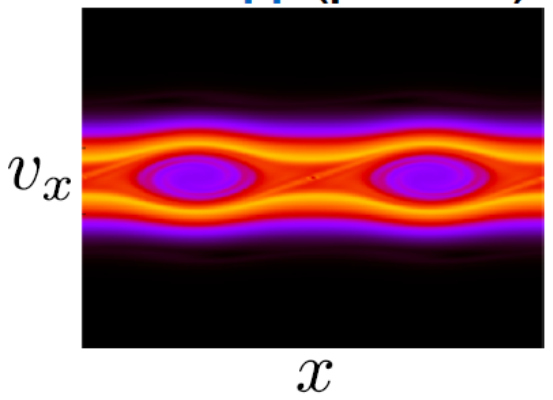
# Development of new 4D mini-applications to encapsulate key GYSELA features → Test the best strategy for next exascale architectures

- Work initiated during Y. Asahi post-doc at IRFM (2017-2018) and pursued by Yuuichi since his return in Japan

**GYSELA (3D torus)** $(r, \theta, \phi, v_{\|}, \mu)$




**Mini-app (periodic)** $(x, y, v_x, v_y)$

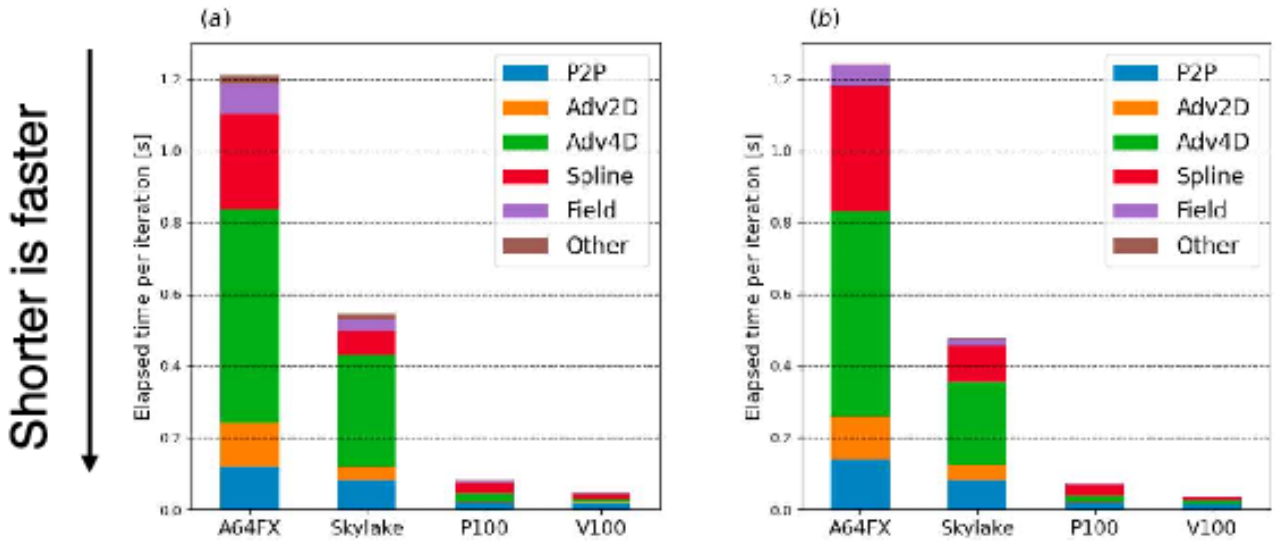



| | GYSELA | Mini-app | Mini-app MPI |
|---|---|---|---|
| System | 5D Vlasov + 3D Poisson | 4D Vlasov + 2D Poisson | 4D Vlasov + 2D Poisson |
| Geometry | Realistic tokamak geoemtry | Periodic boundary conditions | Periodic boundary conditions |
| Scheme | Semi-Lagrangian (Spline) + Operator splitting | Semi-Lagrangian (Lagrange) + Operator splitting | Semi-Lagrangian (Spline) without Operator splitting |
| MPI | Yes | **No** | **Yes** |
| X | OpenMP | **OpenACC/OpenMP/Kokkos** | **OpenACC/Kokkos** |
| Language | Fortran 90 | **C++** | **C++** |
| Lines of | More than 50k | About 5k | About 8k |

*https://github.com/yasahi-hpc/vlp4d*

*Y. Asahi (JAEA/Japan), G. Latu (CEA/DES), J. Bigot (CEA/MDlS)*

# Experience feedback with OpenMP/OpenACC and KOKKOS




| Kernel | A64FX | Skylake | P100 | V100 |
|---|---|---|---|---|
| P2P (Kokkos) | 0.117 [s] | 0.0812 [s] | 0.0189 [s] | 0.0179 [s] |
| Adv2D (Kokkos) | 0.125 [s] | 0.0379 [s] | 0.00275 [s] | 0.00179 [s] |
| Adv4D (Kokkos) | 0.592 [s] | 0.311 [s] | 0.0225 [s] | 0.00730 [s] |
| Spline (Kokkos) | 0.269 [s] | 0.0673 [s] | 0.0277 [s] | 0.0163 [s] |
| Field (Kokkos) | 0.080 [s] | 0.0307 [s] | 0.00729 [s] | 0.00267 [s] |
| Total (Kokkos) | 1.211 [s] | 0.545 [s] | 0.0805 [s] | 0.0468 [s] |
| **Kernel** | **A64FX** | **Skylake** | **P100** | **V100** |
| P2P (OpenMP/OpenACC) | 0.140 [s] | 0.0820 [s] | 0.0191 [s] | 0.0140 [s] |
| Adv2D (OpenMP/OpenACC) | 0.118 [s] | 0.0425 [s] | 0.00350 [s] | 0.00137 [s] |
| Adv4D (OpenMP/OpenACC) | 0.573 [s] | 0.231 [s] | 0.0174 [s] | 0.00925 [s] |
| Spline (OpenMP/OpenACC) | 0.348 [s] | 0.101 [s] | 0.0261 [s] | 0.00982 [s] |
| Field (OpenMP/OpenACC) | 0.0594 [s] | 0.0155 [s] | 0.00470 [s] | 0.00260 [s] |
| Total (OpenMP/OpenACC) | 1.241 [s] | 0.476 [s] | 0.0729 [s] | 0.0378 [s] |

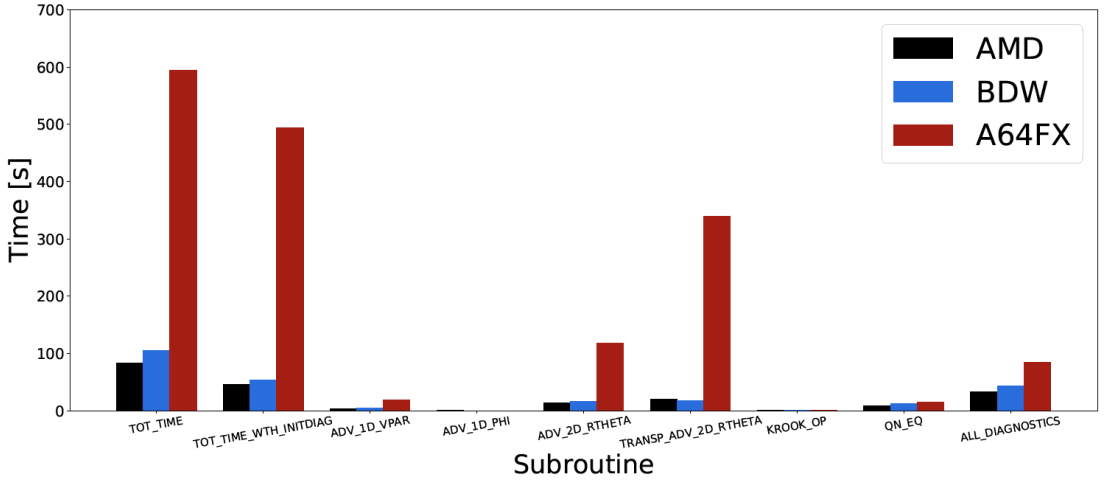
- Directive based approach : mixed OpenACC/OpenMP
  - Mixed OpenACC/OpenMP achieves high performance (marginal on A64FX)
  - Suitable for porting a large legacy code (e.g more than 50k LoC)
  - Intoducing OpenACC View improves the readability
  - SIMD optimizations (like strip-minig) are critical on CPUs

[Y. Asahi et al, to be submitted to P3HPC 2021]

- Higher level abstraction: Kokkos
  - Kokkos can achieve good performance portability except for A64FX
  - Appropriate choice of an execution policy seems critical for CPUs
  - Layout and SIMD tunings improve the performance when cache matters

# GYSELA-X porting on ARM architecture not straightforward

- Comparison between A64FX (FUGAKU/Japan machine) and AMD (TGCC/France machine)




- Total time 7 times bigger on A64FX
- First tests on the ARM partition recently installed at TGCC/France (06-2021) show the same behaviour

- First analysis with Riken team show problem of compiler optimization:
  - Most of the code is not vectorized due to pointer variables
  - The main loop of the routine advec2d is affected by inline-expansion (A function that is not inline expanded becomes a function call. Fujitsu compiler seems to not vectorize do loops that contains function calls)
- Investigation will be pursued via CEA/Riken collaboration + TGCC High Level Support Team
- But currently do not see how to overcome the problem without a strong refactoring of the code

*Riken/Japan : M. Sato, M. Tsuji, T. Odsuya + Y. Asahi (JAEA/Japan)*

# Conclusion & perspectives

- More realistic geometry has been implemented in GYSELA-X
  - First tests with GAM with FKE successful

- Generalized non-equidistant splines successfully implemented in VOICE
  - Next step : Implementation in GYSELA-X → not trivial because impact almost all the code

- PDI successfully implemented in GYSELA-X
  - Restart files can be saved in HDF5 or other formats (as FTI or SionLib, …) to facilitate future I/O tests on exascale machines
  - Next step: Pursue the decoupling of I/O from the computing kernels → coupling with Python + DASK array to perform diagnostic computations

- First porting on new architecture (GPU and ARM) for preparing the code to ITER exascale future simulations
  - In both cases seem to require lots of refactoring to get good performance
  - As the implementation of the non-equidistant mesh to treat strong gradient in the SOL will need strong modification of the code

  → maybe good time to think to a rewriting of GYSELA-X code : Fortran + OpenACC or OpenMP, C++/Kokkos ?