EUROfusion

ACH-HPC-Centers Meeting, 27th / 28th November 2024, Barcelona, Spain

CIEMAT-BSC ACH

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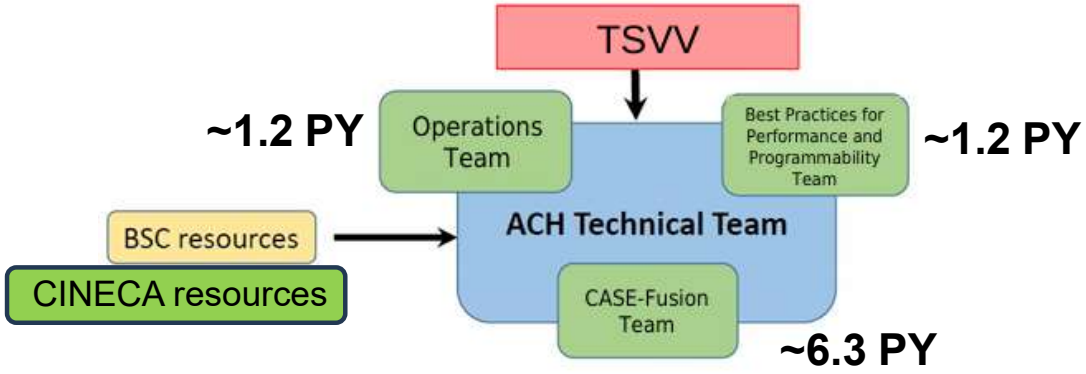
Hub description and involved teams



+ support teams from CINECA and BSC

MARCONI/A100

LEONARDO 4x NVIDIA Tensor Core GPUs

MN4

CTE-AMD 2x GPU AMD Radeon Instinct MI50 with 32GB

MN5 4x NVIDIA Hopper H100 64GB HBM2

BePPP	Programmability, portability, deep performance analysis tools
Operation	Optimization and scalability study Parallelization assistant
Fusion	GPU porting, Parallelization of codes (use of HPC libraries), development of parallel algorithms, performance and scalability analysis.

Professional profiles:

Mathematicians	**10%**
Physicists	**27%**
Computer scientists	**63%**

We work over 12 codes in the period 2021/2024

GPU porting: ERO2.0, X-TORK, BIT1

Code	done	Under development	Next steps
ERO2.0	✓ Identify the more demanding portion of the code ✓ First version over OPENACC recursivity ✗ Second version over standards libraries	● Third version changing the recursivity Octree	◆ Upload the final version to GITLAB ◆ Test of the version in production cases ◆ Increase optimization
BIT1	✓ Identify the more demanding portion of the code ✗ First version using OpenACC in subroutines Arrange.c		◆ Test of the version in medium cases
X-tork	✓ All kinetic related subroutines were ported to GPU using OpenACC. ✓ The fluid part is still working properly. ✓ cc	● **Interpolate_eb_fields** subroutine could not be totally ported since it has a **return** statement inside it ● XTOR-K have to be refactored ● To get rid of such statement ● Reorder some do-loops	◆ First GPU version optimized to be tested in production cases.

General improvements/testing/optimization

Code	done	Under development	Next steps
JOREK	✓ Reduce memory consumption. (SVD)	• Eigenvalues libraries for Big cases. (ELPA)	❖ Upload the SVD solution to the branch of the code.
SPICE2	✓ PESTC solver created ✓ Parallel electric field created	• Create a complete parallel version or spice2	❖ Final version to GITLAB. ❖ IO parallelized
GENE-X	✓ Testing reordering strategies	• Test new demanding cases.	❖ The reordering was study, and the best reordering strategy identified.
SPEC	✓ Performance Analysis		❖ Final work was reached in 2024
BOUT++	✓ Performance Analysis/Optimization		❖ Some portion of the code were tested. ➢ Impossible compile HERMES code.
KNOSOS	✓ Optimization		❖ Openmp final version (2023)
SOLPS	✓ Optimization / Vectorization	• New work for 2025 has been requested	❖ The optimization/vetorization is finalized and tested.
STELLA	✓ Optimization ✓ Reduce memory in the initialisation process.	• Test production cases. • SCALAPACK solver for LU decompositions	❖ The optimization is finalized and tested in small cases.

Achievements

- Only 1 code rejected over the 12 codes received in the period 2021/2024
- For 2025, we will receive two new codes: Alya and GVEC.
- We finished the work for 8 codes (KNOSOS, GENE-X, BOUT++ and SPEC).
- Four of this codes renew the request with new requirements of improvements: JOREK, SPICE2, STELLA and SOLPS.
- We are working in GPU versions for 3 codes. ERO2, BIT1 and X-TORK that are at this moment under development.
- We presented works over 5 workshops and publish 2 papers in PPCF
- We presented a webinar for the code developers with our work (JOREK)
- We maintained more than 54 meetings with developers until now

Some considerations to discuss

- We need to discuss about standardization. Many of this work require (extensive) involvement of the developers. It is important to include them in this discussion (especially for the problems above!).
- Some developers are concerned about the time in supercomputers related to testing and use into the ACH environment. We can propose RES, and be part of the call.
- HPCMI tool.

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Many thanks!