

The French Alternative Energies and Atomic Energy Commission (CEA) From research to industry

Tackling the Arm architecture for the CEA Fundamental Research Division (DRF)

France Boillod-Cerneux - Fundamental Research Division

Numerical simulation deputy

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CEA is part of the french consortium that will apply to the EuroHPC call in order to host and manage the second exascale supercomputer in Europe















- EuroHPC is promoting European technologies, among which the European Processor
 - ☐ The EuroHPC JU aims to:
 - develop, deploy, extend and maintain in the EU a world-leading federated, secure and hyper-connected supercomputing, quantum computing, service and data infrastructure ecosystem;
 - support the development and uptake of demand-oriented and user-driven innovative and competitive supercomputing system based on a supply chain that will ensure components, technologies and knowledge limiting the risk of disruptions and the development of a wide range of applications optimised for these systems;
 - widen the use of that supercomputing infrastructure to a large number of public and private users and support the development of key HPC skills for European science and industry.



- In this context, CEA is focusing on Arm based supercomputers in order to tackle target technologies
 - Among which Rhea and Cronos



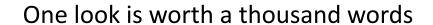


- CEA is a member of EUPEX project (EuroHPC) which will provide
 a prototype of future European Exascale supercomputers
 - Prototype blades with Rhea CPUs
 - Two CEA applications are embedded within EUPEX
 - ☐ Sun modelling and material science applications









GPUs



Arm

Data

Scalability

Our applications





exascale



- cea
 - Application community in France is mobilized in order to anticipate the execution of our applications on European architectures
 - CEA, CNRS, Inria and France Universities joined together to identify the spectrum of our HPC, AI, HPDA and HTC applications



- The objectives are to understand clearly what
 - Is the current state of the applications? (GPU enable? Arm enable? Current scaling? EU, international community?)
 - Are the objectives of the applications towards Exascale computing (scientific case and expected scalability)
 - Are the human resources necessary to achieve the Exascale objectives
 - Want to contribute? Mail me! <u>France.boillod-cerneux@cea.fr</u>

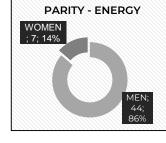
 Report (in french) is available at CEA's booth

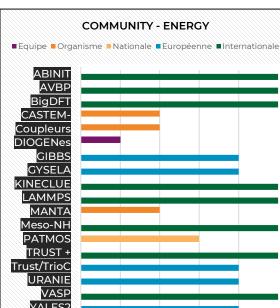
230 researchers involved

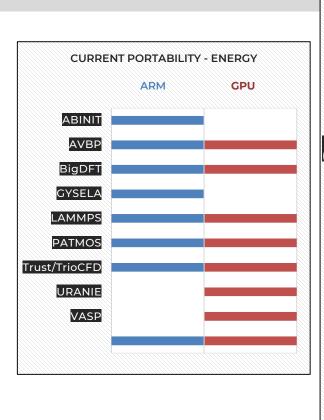


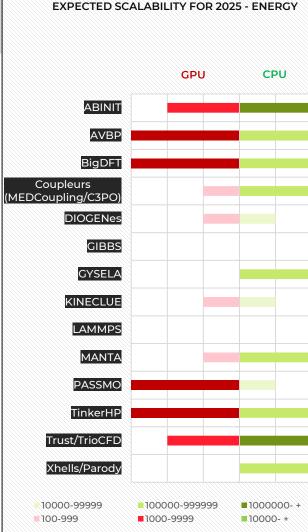


ENERGY APPLICATIONS











GYSELA-X is a semi-Lagrangian code addressing gyrokinetic full-f global simulations of flux driven tokamak plasmas



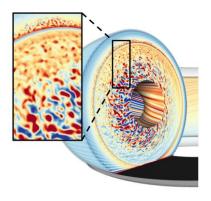
Ongoing collaborative work with Atos, Arm and RIKEN to execute efficiently GYSELA on Fugaku and joliot-curie supercomputers

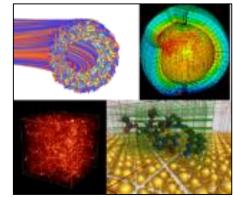


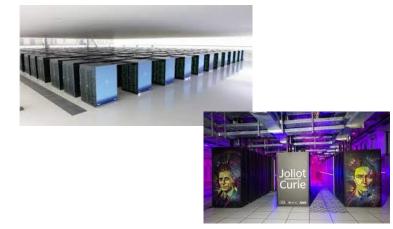
Atos







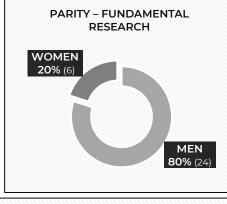


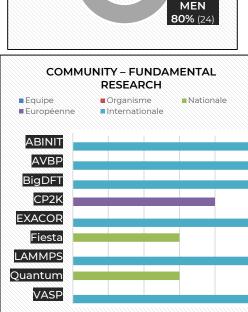


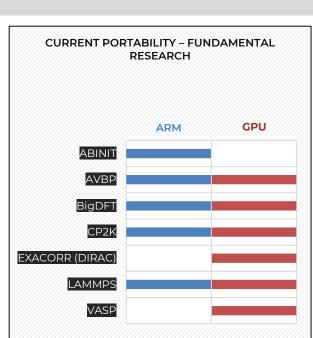


FUNDAMENTAL RESEARCH APPLICATIONS

CEA)







FUNDAMENTAL RESEARCH

ABINIT

AVBP

BigDFT

CP2K

EXACORR (DIRAC)

10000-99999

100-999

Fiesta beDEFT

LAMMPS

GPU



EXPECTED SCALABILITY FOR 2025 -





CPU



















































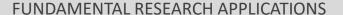
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 BigDFT is a fast, precise, and flexible DFT code for ab-initio atomistic simulation. With BigDFT, atomistic modeling is more powerful and accessible



- BigDFT is able to tackle large Arm supercomputers
 - Running on A64FX architecture
 - ThunderX2 architecture
 - Collaborative work with



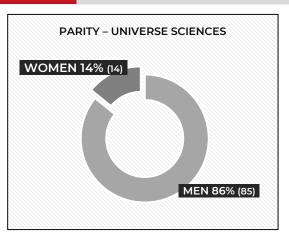


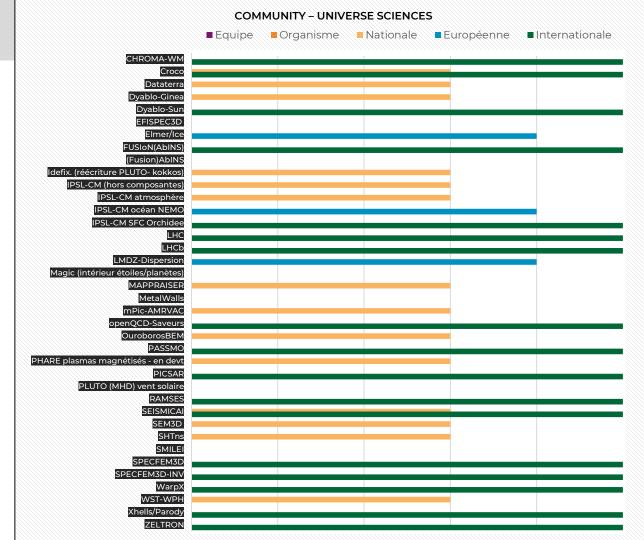




 Collaborative work on Covid19: Fugaku has been exploited by BigDFT to perform full quantum mechanical modeling of the main protease of the SARS-CoV-2 virus in complex with a large database of potential inhibitors







UNIVERSE SCIENCES APPLICATIONS

cea

CURRENT PORTABILITY - UNIVERSE SCIENCES GPU ARM CHROMA-WM Croco Dyablo-Ginea Dyablo-Sun EFISPEC3D FUSION(AbINS) Idefix. (réécriture PLUTO- kokkos) IPSL-CM (hors composantes) IPSL-CM atmosphère IPSL-CM océan NEMO LHC LHCb LMDZ-Dispersion Meso-NH openQCD-Saveurs OuroborosBEM PHARE plasmas magnétisés - en PICSAR PLUTO (MHD) vent solaire RAMSES SEISMICAI SEM3D SEM4Exascale SHTns SMILE SPECFEM3D SPECFEM3D-INV WarpX WST-WPH Xhells/Parody ZELTRON

EXPECTED SCALABILITY FOR 2025 – UNIVERSE SCIENCES





Warpx is an open-source Particle-In-Cell code for the exascale era















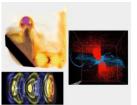












Running pretty well on A64FX: Finalists to the ACM Gordon Bell award for SC22

CEA: Luca Fedeli, Neil Zaim and Henri Vincenti;

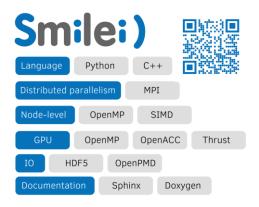
RIKEN: Miwako Tsuji, Hitoshi Murai & Mitsuhisa Sato;

Partners: Atos, GENCI, Arm and Fujitsu





- Smilei is an open-source multi-physics massively parallel scientific application designed to simulate a broad range of plasma physics scenarios
- The code is built around the standard Particle-In-Cell method enriched by many additional physical modules: particle collision, ionization, nuclear reactions, synchrotron-like radiation, strong-field quantum electrodynamics (SF-QED) processes (via Monte-Carlo procedures).













 Dyablo dyablo is a new simulation code developed at CEA in Saclay for the modelling of magnetohydrodynamics on AMR grids

To reach exascale performances, the code relies on the portability performance library Kokkos to do shared parallelism while distributed parallelism is done using MPI









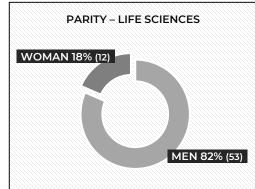


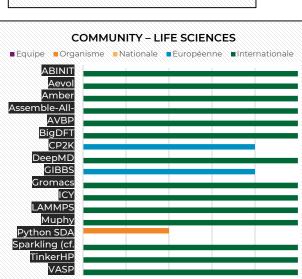


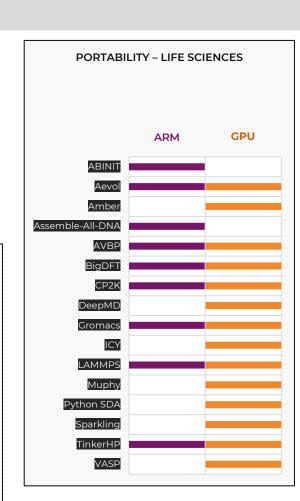


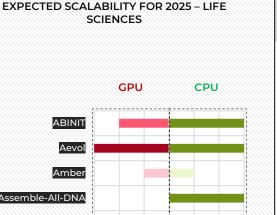


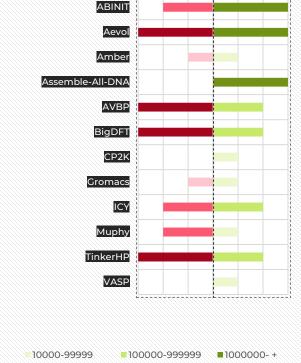












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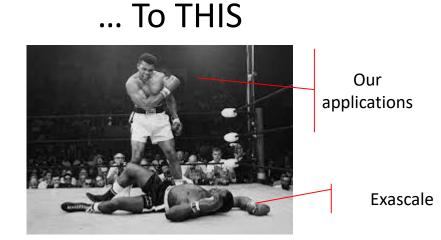
- Gather the scientific community to accelerate the ongoing work around applications portability
 - Arm architectures
 - GPU architectures
- Academic & industrial researchers, we need you!







Exascale







- Environment and Climate modelling (hpc hpda ia)
- Neurosciences (hpda ia)
- Laser/matter interactions, plasma modelling (hpc)
- Material sciences (hpc hpda ia)
- Astrophysics and cosmology (hpc hpda ia htc)
- Nuclear Physics and high energy physics (htc ia)
- Drug design(hpc hpda ia)
- Omics (htc hpda ia)
- Fusion energy (hpc ia)
- Might have forgotten some more applications...



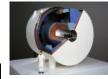








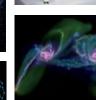










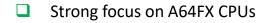


- Open science
- National, European or international applications
- (a lot of) real/observational data

COLLABORATIONS AROUND ARM ARCHITECTURE

- Anticipate future architectures so we can execute our applications on future European exascale and post-exascale supercomputers
- Regular exchange and work with Arm experts and RIKEN researchers





- Thanks to a bilateral CEA-RIKEN collaboration, CEA's researchers can access Fugaku supercomputer
- Long term collaboration (since 2017)











