ANNUAL REPORT

2021

GENCI

HPC at the service of knowledge

GENCI

GENCI is responsible **to provide very large scale computing and massive data processing resources,** at the national and European level, for **promoting the use of HPC and Artificial Intelligence** among both academic and industrial open research communities.

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www.genci.fr

3 COMPUTING CENTERS, FOR A TOTAL OF 54.6 PFLOP/S

CINES
OCCIGEN supercomputer
3.5 PFLOP/s - 555 million hours allocated

IDRIS
JEAN ZAY supercomputer
28.3 PFLOP/s - 508 million hours allocated

TGCC
JOLIOT-CURIE supercomputer
22 PFLOP/s - 1.412 billion hours allocated

5 SHAREHOLDERS

MINISTÈRE DE L'ENSEIGNEMENT SUPÉRIEUR, DE LA RECHERCHE ET DE L'INNOVATION
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GENCI AT THE HEART OF THE BIGGEST CHALLENGES

FOREWORD BY CLAIRE GIRY

**DIRECTOR GENERAL FOR RESEARCH AND INNOVATION,
MINISTRY FOR HIGHER EDUCATION, RESEARCH AND INNOVATION**

2021 is definitely an important year with the upcoming arrival of new computing resources at CINES, and with an increase in GPU power at IDRIS, funded through the national AI strategy. GENCI is at the heart of several national strategies: artificial intelligence, quantum technologies, and finally the cloud. GENCI is also coordinator of an Equipex+ project bringing together several computing and data processing Tier2 structures disseminated throughout the country.

At European level, and building on this solid foundation built in 2021, GENCI is preparing an application to host an exascale supercomputer at the TGCC, during a call to be launched by EuroHPC in 2022.

More than ever, GENCI is strengthening its role as France's computing operator for research and innovation.

JEAN ZAY at IDRIS

© CNRS - Cyril Fresillon

© CEA - Painting: C215

JOLIOT-CURIE at TGCC (CEA)

© CINES

OCCIGEN at CINES

EDITORIAL BY PHILIPPE LAVOCAT

CEO OF GENCI

Despite a very restrictive 2021 health situation, GENCI kept on developing its activity at the service of scientific and industrial research communities in its regional, national and European dimensions. Here are some highlights.

GENCI continued to provide support to research teams in the fight against COVID19: around thirty projects ran efficiently in 2021 on our computers! GENCI equipped IDRIS and CINES with valuable storage resources, and signed the contract for the acquisition of the Adastra computer which will be operational at CINES in autumn 2022. Pursuing its mission to implement the national strategy in Artificial Intelligence, via the Jean Zay calculator operated by IDRIS, already a great success with nearly 600 AI projects in the year, GENCI has launched an operation to increase its capacities: Jean Zay3 will be operational at the beginning of 2022. GENCI should thus have a computing power of more than 130 PF from the 3 centers by autumn 2022.

Selected in the PIA3, the MesoNet project, piloted by GENCI, forerunner of a distributed infrastructure of regional mesocentres, started in the fall. Sensitization of SMEs to digital simulation continued via SimSEO within the framework of the National HPC Competence Centers and the relationship with industry was developed through proofs of concept, within the framework of the quantum programs of the Ile-de-France Region.

The growing European action of GENCI has manifested itself in strategic projects for France; participation in setting up the EUPEX project selected by EuroHPC, demonstrator of the future European computing architecture which will be used in the exascale machine to be hosted and operated by France at the TGCC in 2024. EUPEX relies on the EPI initiative, aimed at developping a European processor, in which GENCI acts as an interface between the scientific communities and the designers in the co-design launched on a European scale. Quite logically, the major action of the year was the establishment and start of the organization of the Exascale-France Project and the search for national and European partners to create a consortium with a view to applying for the call for interest of EuroHPC which will be launched in the spring of 2022. Representing France on the Council Board of PRACE, GENCI has also been a driving force in the establishment of close collaboration between EuroHPC and PRACE relating, among other things, to the selection process projects to access the computing hours of EuroHPC machines. GENCI is proud to have been able to provide its technical expertise to the French Ministries involved in the governance of EuroHPC.

> // GENCI now offers its Associates' teams a range of strategic tools integrating intensive computing, artificial intelligence, and the beginnings of quantum technologies. //

Finally, 2021 saw the materialization of intense investment work in the examination of new projects in response to the strategic requests of its Partners, within the framework of the National Quantum Plan: GENCI signed on December 1 with EuroHPC an agreement starting the European project HPCQS, hybrid HPC and quantum infrastructure. The latter will serve as a fundamental building block to start the PNCQH program, the future National Hybrid Quantum Computing Platform, for which GENCI was selected with its Partners as part of the French PIA4 calls for projects.

In 2022, the French Presidency of the European Union will emphasize digital sovereignty: GENCI now offers its Associates' teams a range of strategic tools integrating intensive computing, artificial intelligence, and the beginnings of quantum technologies. All these exciting subjects developed in this issue are due to the tireless investment of the team associated with those of the computing centers. The fruitful cooperation with our Associates thus offers very encouraging prospects for the future. ■

2021 AS SEEN BY GENCI'S SHAREHOLDERS

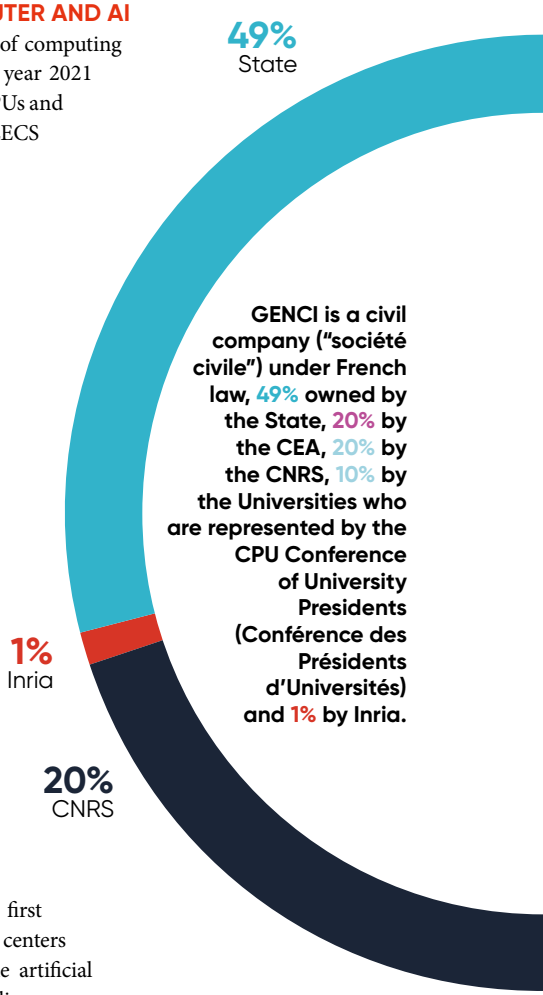
Jean-Frédéric Gerbeau
DEPUTY CEO FOR SCIENCE AT INRIA

Inria

–– AN INTEREST FOR THE JEAN ZAY SUPERCOMPUTER AND AI

GENCI and Inria were chosen in 2020 to receive a donation of computing resources from AMD to support research into Covid19. The year 2021 saw the installation of a system, equipped with AMD EPYC GPUs and AMD Instinct Accelerators, in the national GRID'5000/SILECS infrastructure on the ENS Lyon site.

Besides, in 2021, the Inria project-teams have confirmed their interest in the Jean Zay supercomputer. Its adoption for AI work has led to a very significant increase in Inria's use compared to what was observed in classic HPC simulation. The profile of Inria users has changed considerably in a very short time. The new procedures put in place to access the machines are particularly appreciated. ■



GENCI is a civil company ("société civile") under French law, 49% owned by the State, 20% by the CEA, 20% by the CNRS, 10% by the Universities who are represented by the CPU Conference of University Presidents (Conférence des Présidents d'Universités) and 1% by Inria.

Denis Veynante
DEPUTY DIRECTOR WITH RESPONSIBILITY FOR DIGITAL INFRASTRUCTURES WITHIN THE RESEARCH OPEN DATA DEPARTMENT, CNRS

cnrs

–– AN UNFAILING COMMITMENT OF OUR TEAMS

The deployment and extensions of the Jean Zay computer, the first converged architecture in Europe, marks the arrival in national centers and the world of high-performance computing (HPC) of the artificial intelligence (AI) community and its applications. The extraordinary success of the machine with this community is now reflected in more projects involving AI than HPC. The unfailing commitment of the IDRIS teams, whose workload has increased significantly in the service of users, was honored by the awarding of a CRISTAL Collectif by CNRS

At the same time, the dynamics involving IDRIS, CNRS and GENCI is confirmed with the success of the CLUSSTER project, coordinated by ATOS and with the participation in particular of Qarnot Computing, OVH and Inria, to develop a research cloud for AI. ■

–– GREAT PERSPECTIVES FOR 2022

By 2020, Genci and the TGCC were thoroughly committed to provide priority access to computational resources to research teams involved in the fight against COVID-19. These efforts have paid off. Researchers from the Fundamental Research Division of CEA, took part in a large international collaboration to study how SARS-COV-2 proteins are synthetized. Part of the calculations (40 Mh) was executed on the AMD partition of the Joliot-Curie machine and the modeling contributed to the development of new antiviral drugs.

Thus, 2021 stands out as a very good year in the HPC ecosystem at both European and national levels. With Genci, the CEA has been successfully involved in several EuroHPC calls for projects. As part of the quantum plan, the TGCC has been chosen to host the first machine of the National Platform for Hybrid Quantum Computing, combining both classical supercomputers and the first quantum accelerating devices, opening up great perspectives for 2022.

Maria Faury
DIRECTOR FOR INTERNATIONAL AND LARGE SCALE INFRASTRUCTURES RESEARCH CEA/DRF

–– A DYNAMIC AND EFFICIENT ACTIVITY

GENCI's activity in 2021 was particularly dynamic and efficient. In particular, it directly involved France Universities (formerly CPU) with the procedure to replace the OCCIGEN machine at CINES, which will be effective in 2022, and the coordination of the MesoNet project, which brings together a large number of mesocentres coming from our organizations. But the scientific community of members of France University has also been strongly mobilized within the framework of GENCI's technology watch unit in the service of the project to acquire and host an Exascale machine in France to meet scientific challenges, societal and economic issues posed by supercomputing. Finally, thanks to the collective dynamics of the national centers led by GENCI, significant changes have been made very quickly in the method for allocating computing hours to meet, on the one hand, the new needs of users in the field of artificial intelligence and, on the other hand, to the urgency posed by the launch of research projects dedicated to COVID19 carried out by our organizations. The challenges of digital technology are considerable and affect in particular all aspects of the missions and operation of universities.

Guillaume Gellé
PRESIDENT OF THE REIMS CHAMPAGNE-ARDENNE UNIVERSITY / PRESIDENT OF THE CINES BOARD OF DIRECTORS / PRESIDENT OF THE CPU UDUCATION COMMISSION

Within this general framework, since its creation, GENCI has played an essential role in the construction of a national ecosystem to meet the computing and data processing needs of the entire scientific community and has been able to evolve constantly to take up new subjects such as Big Data, artificial intelligence or quantum computing.

FOREWORD BY RENAUD VEDEL

COORDINATOR OF FRANCE'S NATIONAL AI STRATEGY

Incepted after a proposal of the Villani Report, the AI partition of the Jean Zay supercomputer must be considered both a pillar and a success of the first phase of the national strategy for AI.

Over the last 5 years, the number of scientific publications integrating AI has increased sixfold in the ArXiv library.

With its 1,000th project supported after only 2 years, GENCI has demonstrated, with the support team and the network of CNRS and Inria research engineers, how much it was contributing to the fast dissemination of the methodological tools that contemporary AI brings to the widest variety of French sciences.

> // GENCI has demonstrated how much it was contributing to the fast dissemination of the methodological tools that contemporary AI brings to the widest variety of French sciences. //

With its support for the exceptional international natural language processing project called BigScience, GENCI is demonstrating its power of attraction in the service of open science.

With its ability to support numerous French companies and startups for projects leading to publication, GENCI contributes to the growth of the French economic ecosystem in AI through public-private partnerships.

Moreover, we are already assured that 2022 will be marked by the achievement of new challenges and the completion of new projects, accelerated by the dynamism and communicative warmth that emanates from GENCI.

The major expansion of Jean Zay's computing capacity and new shared services for the French AI community are on the agenda. There is no doubt that GENCI will be there to support the new research program on embedded AI, decentralized AI, trusted and frugal AI and the mathematical foundations of AI, financed by the French government as part of "season 2" of the National Strategy for AI!

WHAT THEY SAY ABOUT US!

CEA, CINECA AND GENCI: HAND IN HAND TO REACH THE EXASCALE

The heads of the three research centres (two French and one Italian) have signed a joint commitment: this memorandum of understanding aims to mobilise these three major players in the field of digital science to work together on the road to exascale and post-exascale computing. It provides a framework to record the common interests of the parties to join forces in the framework of the actions/initiatives launched by the EuroHPC Joint Undertaking and to define the way to prepare a long-term collaboration agreement, explains the CEA. To begin with, this agreement aims to involve the parties in the response to the call for applications to host a European exascale computer and future calls for applications for the development of new European processors or a European software stack.

nextinpact.com

Italy and France join forces towards the Exascale: what is it and what will it be used for?

In the wake of the Quirinal Treaty signed a few weeks ago in Rome by Presidents Sergio Mattarella and Emmanuel Macron, Italy and France are getting closer and closer. Also in the field of scientific research.

corriere.it

FOREWORD BY NEIL ABROUG

HEAD OF THE FRENCH NATIONAL QUANTUM STRATEGY

The "France 2030" is a unique opportunity to address the major international challenges of today, including quantum technologies. In order to position France among the leading nations mastering such technologies, the French President has launched on 21 January 2021 a national strategy toward quantum technologies.

In order to avoid a strong dependency to a single operator and to answer to French ambitions in terms of NISQ computers and software solutions, the French government asked to CEA, GENCI and Inria to install at TGCC an hybrid HPC/Quantum platform with the following goals:

- Take benefits from existing quantum accelerators and integrate them into the broader context of high performance computing and developing hybrid quantum-classical algorithmic solutions
- Disseminate the use of quantum computing in priority sectors by developing software solutions and hardware-agnostic development environments based on programming languages and libraries dedicated to different application sectors.

Indeed, through its missions to equip French computing centres and the use of a unified national policy for the allocation of computing hours for scientific users of high-performance computing, Genci has acquired recognised expertise, including at European level. This recognition can be seen in its participation in the implementation of the first pan-European hybrid quantum computing infrastructure (HPC + quantum) in the framework of the HPCQS consortium, which was selected by the EuroHPC JU and which will be one of the pillars of the French platform.

For these reasons, the government decided to entrust Genci within the national platform with the acquisition and dissemination aspects, while the R&D aspects would be managed by CEA and Inria.

Evaluated positively by a committee of international experts, the government validated the work programme proposed by CEA, GENCI and Inria at a ceremony organised at Institut d'Optique Graduate School (IOGS) on 4 January 2022.

> // The French government asked to CEA, GENCI and Inria to install at TGCC an hybrid HPC/Quantum platform. //

Jean Zay, the supercomputer that (also) loves AI

AI is becoming ever more demanding and needs supercomputers. While meeting the classic needs for intensive computing, the Jean Zay equipment offers a response adapted to the heavy applications of AI. It is intended to be the precursor of an announced convergence between HPC and AI.

dataanalyticspost.com

Why the Jean Zay supercomputer is experiencing an increase in its performance in artificial intelligence

The Jean Zay supercomputer is at the heart of several cutting-edge research projects such as Big Science. It has become an essential tool and ActuIA has also devoted an article to it in the next issue of the magazine, which will be published in a few days.

actuia.com

ADASTRA : A NEW FRENCH SUPERCOMPUTER ON THE ROAD TO EXASCALE

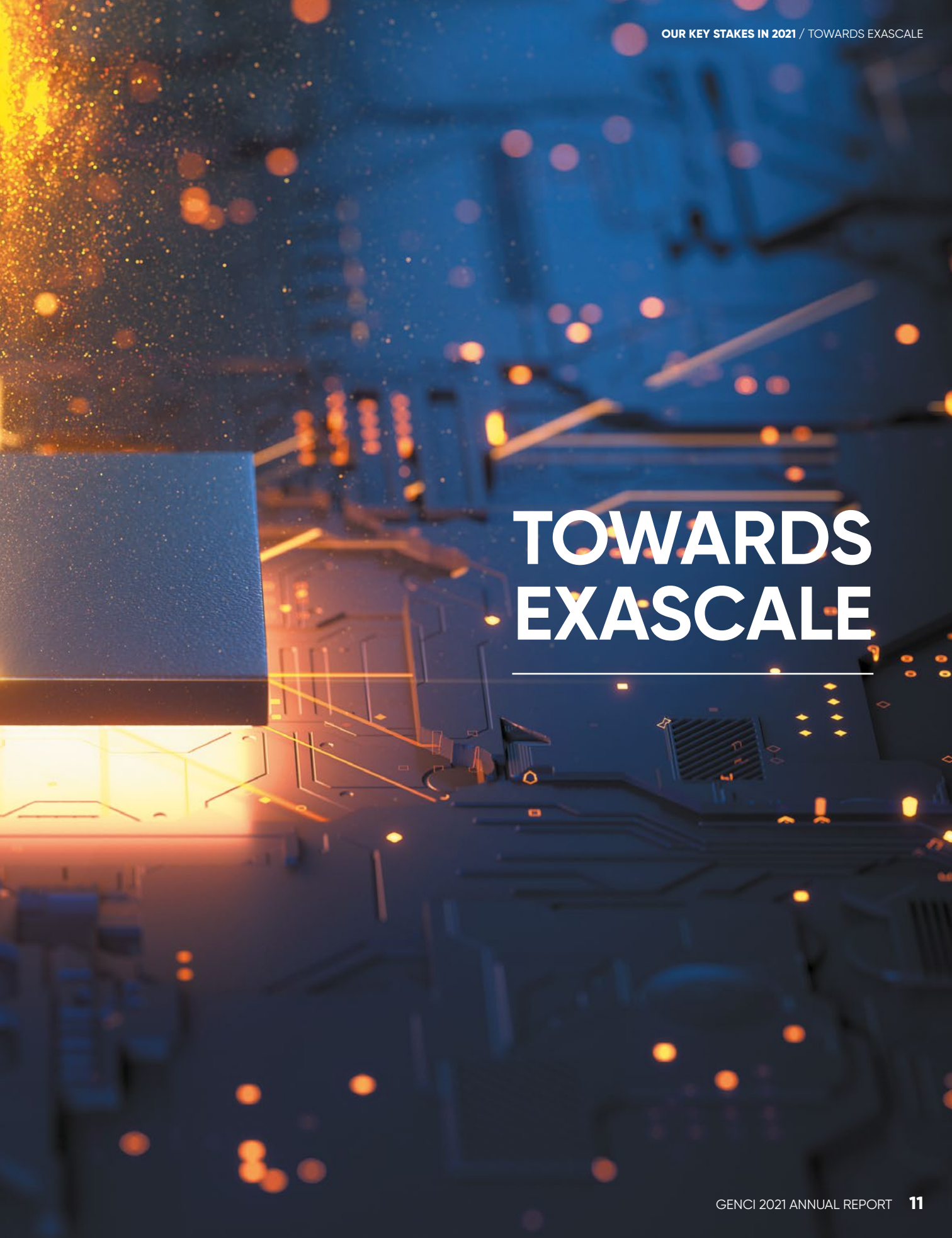
At 2022 horizon, Adastra will be one of the most powerful supercomputers for academic and industrial open research in Europe, thanks to its state-of-the-art architecture, which will complement GENCI' systems already available at the two other national computing centers (TGCC for the CEA and IDRIS for the CNRS-INS2I).

genci.fr

MORE INFO

www.genci.fr

OUR KEY STAKES IN 2021



TOWARDS EXASCALE

EUROHPC: EUROPE TOWARDS EXASCALE

Created in 2018 and located in Luxembourg, the EuroHPC Joint Undertaking (currently consisting of European Commission and 34 Member States) began a second mandate in 2021 with the adoption in July of the regulation defining its mode of operation and its priority objectives for 2021-2027.

After setting up a pan-European computing infrastructure aggregating 5 multi-class Petascale systems and 3 pre-Exascale systems, EuroHPC is turning to the next stage of its deployment: exascale. An exascale-class supercomputer is at least twice as powerful as the most powerful system funded to date by EuroHPC and is comparable to those recently put in operation in Japan, China and the United States.

The EuroHPC roadmap plans the acquisition of 2 exascale class supercomputers, one in 2023 and one in 2024 which will be hosted by entities selected in 2022 and 2023.

For this purpose, GENCI and its associates and in particular the CEA which will host this supercomputer at the TGCC are preparing their application for the 2nd Exascale call for expressions of interest expected in 2022.

For this in 2021:

- contacts have been launched with potential national (academic and industrial) and international partners to ensure co-financing of 50% of the Total Cost of Ownership based on 5 years of operation of the supercomputer;
- the architecture (computing, storage, IT environment) that could compose a converged Exascale machine (HPC, IA and HPDA) has been developed, using scalar resources but above all accelerated resources and possibly integrating for some targeted applications quantum accelerators;
- the needs of the user scientific communities have been identified and assessed in terms of application development, support and training.

EuroHPC roadmap plans the acquisition of 2 exascale class supercomputers, one in 2023 and one in 2024.

EXASCALE, GENCI IS PREPARING

BY CHRISTINE MÉNACHÉ
HEAD OF TGCC (CEA CENTRE HOSTING THE JOLIOT-CURIE SUPERCOMPUTER)

In 2021, in addition to the system administration and operation of the four Joliot-Curie computing partitions and their environment, the CEA/TGCC teams were mobilised to carry out the technical studies for the *Exascale France* project.

The TGCC team in front of thé Joliot-Curie computer.

Indeed, it was necessary to produce «pre-project» studies at the facility level (electricity, cooling, structural work, etc.) for the different budget scenarios, in order to confirm the technical feasibility of hosting the computer and its environment. At the same time, scenarios for the urbanization of the TGCC computer rooms have been elaborated in order continue Joliot-Curie operation as long as possible, at least partially. Numerous analysis and projections for the definition of the Exascale computer architecture and its storage environment have been performed, according to the possible electric power supply of the machine. This work should continue in 2022.

In order to allow researchers to start working on the ARM architecture (one of the possible architectures for Exascale), Joliot-Curie's A64FX partition was opened to all national users in early October 2021. Since June 2021, this partition has been reserved for members of the technology watch unit.

A noteworthy fact regarding the life of the computing centre is the setup, end of 2021/beginning of 2022, of new teams for the hotline, and for the operation and management of servers and networks.

The Joliot-Curie A64FX partition open to all national users.

MORE INFO ON OUR WEBSITE

www.genci.fr

THE PRECURSOR MACHINE **OF CINES**

BY BORIS DINTRANS
DIRECTOR OF CINES (CPU CENTRE HOSTING THE OCCIGEN SUPERCOMPUTER)

The year 2021 ended with the end of the joint procedure between GENCI and CINES for the renewal of the Occigen supercomputer, in production since 2015.

After 18 months of exchanges between all vendors during the competitive dialog, the solution provided by HPE have been selected. Called Adastra, this >70 PFlop/s peak performance system, 20x than Occigen, will be one of the most powerful systems for academia and industrial open research in Europe.

Its name Adastra, coming from Latin expression *Per aspera ad astra,* will bring to researchers massive and innovative computing capacities for their complex needs in numerical simulation. It relies on a HPE Cray EX converged system made par AMD Genoa CPUs and MI250X GPUs offering the best TCO (total cost of ownership), a good balance between sustained performance, energy efficiency for a pertinent set of production-based scientific and industrial applications. Additionally, a 2-year innovative collaboration called "contract of progress" has been initiated in November 2021 between HPE, AMD and CINES teams for porting to GPUs 5 real applications in the goal of being ready for the availability mid-2022 of the accelerated partition of Adastra. The complete CPU+GPU system will be fully in production end of 2022, ready for the A13 call for proposals of GENCI, reinforcing the position and the means available to French researchers on this fascinating road to Exascale !

The HPE Cray solution chosen for renewing the OCCIGEN supercomputer.

© HPE

FRANCE LAUNCHES ITS **HYBRID HPC QUANTUM INITIATIVE**

One year after the announcement by the President of the Republic of France of the National Quantum Plan, the coordinator of the national quantum strategy has launched HQI (France Hybrid HPC Quantum Initiative), an academic and industrial research program that will rely on the acquisition of several quantum technologies. These systems will be coupled to GENCI's European-class supercomputer Joliot Curie hosted and operated by CEA, thus serving the interests of French and European researchers as well as international collaborations for open research. This quantum/HPC hybridization is an innovative and unique initiative that will benefit from the expertise of the CEA/TGCC teams in infrastructure operation, security and support to scientists.

With a budget of €72.3 million, this program is managed by the CEA. The SGPI (Secrétariat général pour l'investissement) has entrusted GENCI with the acquisition of simulators and quantum computers for an amount of €36.3 million, which should be supplemented by European and industrial co-financing. The open and scalable platform, will have a set of complementary French and European technologies to best address research issues and business use cases. The second part of the research program has a budget of €36 million. It is led by the CEA and Inria, with the support of the CNRS and France Universities, as well as the sovereign player OVHcloud, the IT manufacturer Atos and startups. Together, they will support the development of a programming and execution software layer on hybrid computing resources, including libraries for business verticals (health, chemistry, finance, etc.) or transversal verticals (machine learning, optimization, etc.). GENCI will be responsible to provide and promote the use of HQI's quantum computing resources as well as the dissemination to the quantum ecosystem. (Le Lab Quantique, QuantX, Teratec, Systematic, etc.), local authorities and industry.

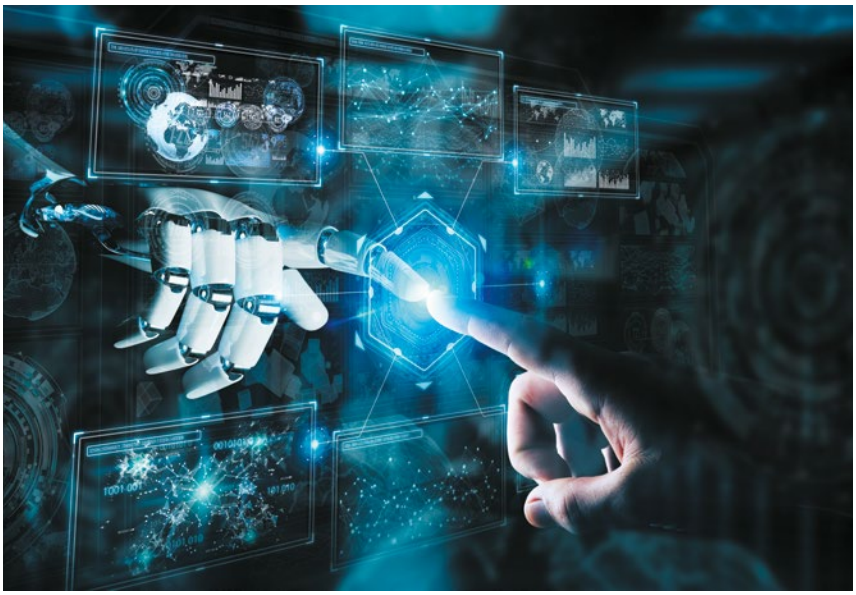
The first component of HQI is already up and running: it is based on the HPCQS project, co-financed by the EuroHPC Joint Undertaking and the 6 member states of the consortium (grant agreement No. 101018180), including France and Germany. France should capitalize on this program and could couple its future Exascale supercomputer with quantum computing resources, paving the path to new computing architectures to address stakes linked to performance/eco-responsibility issues and support users in their journey towards the post-Exascale era.

FRANCE HYBRID HPCQUANTUM INITIATIVE

ARTIFICIAL INTELLIGENCE AND JEAN ZAY

GENCI'S CONTRIBUTION TO THE « AI FOR HUMANITY » PLAN

In response to the announcement in March 2018 of the *"AIForHumanity"* strategy by the French President, GENCI have been charged to implement one of the recommendations toward the provision of sovereign HPC facilities for French researchers in Artificial Intelligence (AI).



In 2019 the converged supercomputer Jean Zay, honoring the name of a former Ministry of Research and co-founder of CNRS before the 2nd world war, has been installed at IDRIS (CNRS). Converged, since its modular hardware and software architecture allows Jean Zay to answer to the needs of both numerical simulation and AI.

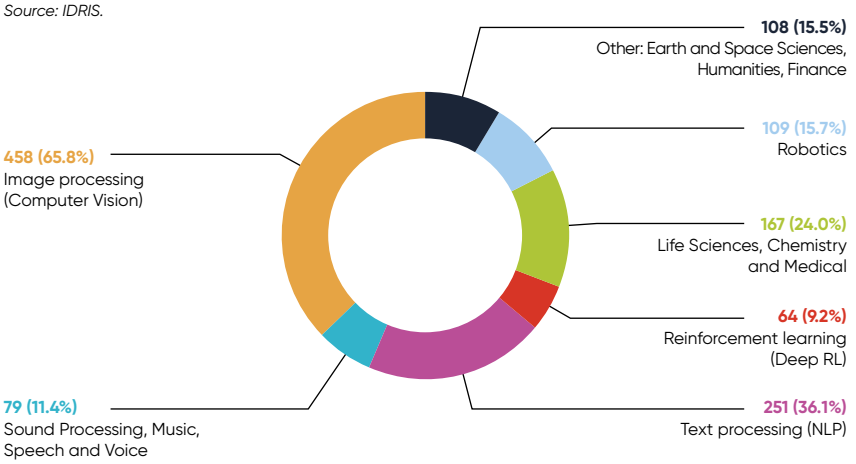
In order to support researchers in taking benefits from Jean Zay, the user support team of IDRIS has been reinforced by **10 additional AI experts coming from CNRS and Inria.**

Two years after its commissioning end of 2019, more than **800 projects in IA have been granted on Jean Zay,** coming from research laboratories (CNRS, Inria, CEA, Universities, INSERM, INRAE, IFREMER, IRCAM, IRD…), startups (more than 30) or large industrial groups ((Renault, Stellantis, VALEO, Orange…) at a ratio of 2 new projects per day! Beyond these numbers Its important to notice the wide variety of AI domains addressed by Jean Zay, with projects in vision, natural language processing, decision-making, smart cities, health/medicine (with some COVID19 related ones), neurosciences, robotics, humanities, chemistry, particles physics, astrophysics, climate research…

At date our Jean Zay supercomputer at IDRIS, installed in the field of #AIForHumanity, **is one of the biggest converged super-computers in Europe,** ready to address the **future challenges of the second round of the French strategy.**

MORE INFO ABOUT
AI FOR HUMANITY
www.aiforhumanity.fr

NUMBER OF FILES BY AI APPLICATIONS
(OUT OF 696 FILES)
Source: IDRIS.



JEAN ZAY BOOSTER

BY PIERRE-FRANÇOIS LAVALLÉE
DIRECTOR OF IDRIS (CNRS CENTRE HOSTING THE JEAN ZAY SUPERCOMPUTER)

Two year and a half after its commissioning, it's time to make a first assessment of the Jean Zay supercomputer.

First national accelerated architecture, the configuration of Jean Zay has been several times extended now reaching a peak performance of 28 Pflop/s (2712 GPU V100). The agreement firmed in February 2021 between CNRS and the EPAPS for reusing the calories generated by Jean Zay within the Paris-Saclay urban campus heat network (equivalent to the heating of 1,000 homes) should be operational in 2022, reinforcing the already remarkable eco-responsible nature of the computer. First national infrastructure dedicated to the Artificial Intelligence community, Jean Zay has been rapidly adopted using the dynamic Access modes (AD) by more than 1000 accounts open (45% of the total number of users) and more than 800 projects (70% of the total number of projects). The tailored user support initiated in 2020, with a dedicated IA team, is composed now by 12 experts (CNRS, Inria) is for sure one of the key elements of success.

Mechanically, this results in a saturation of the resources devoted to AI, further amplified by the emergence of large-scale projects such as the BigScience collaboration in the field of natural language processing.

In parallel, the use of the GPU resources by the HPC community (essentially from CT4, CT7 and CT9) is growing steadily over the months. In order to answer to this demand, the French Ministry of Research granted a new extension of Jean Zay with 8 Pflop/s additional, composed by 52 octo-GPUs A100 80 GB HPE nodes, which will be made available in two phases, first for the BigScience collaboration from February 2022, then for all users from May.

The Jean Zay computer at IDRIS.

© CNRS - Cyril Fresillon

AI AT THE HEART OF SOCIETAL ISSUES

BigScience: a very large, open and multilingual language model

The BigScience project gathers more than 900 researchers worldwide around a shared goal: **the creation and the study of a large-scale language model et its associated dataset.**

A major part of current progresses lies on the use of bigger and bigger languages models trained on even bigger amount of texts.

This race to gigantism is now led within a close context by few actors from the private sector domain which poses issues in many domains: environmental, societal, ethics and access for research purposes.

BigScience shows that another way to create, understand, study and share such results is possible; open science, collaborative, holistic and maximizing the benefits for all parties.

The first results of BigScience have been published in October 2021 with the T0 model and the P3 dataset. **They demonstrate already generalization performances greater than OpenAI' landmark model GPT3, using a 16x smaller model.** In parallel, works on the creation and the open availability of the dataset are progressing well and first related publications have been performed using textual data related to North Africa and Middle East dialects. The final model and dataset will be multi-lingual, the objective is to cover a major part of the more spoken languages in the world. Finally, tools for analysis and evaluation of models have been also made available as part of the works done by BigScience.

MORE INFO ON THE WEB

bigscience.huggingface.co

OPTIMISING THE ANALYSIS TOOLS OF MEDICAL IMAGES

The **optimisation of the analysis tools of medical images of lung radiography** thanks to artificial intelligence techniques, driven by Emilie Chouzenoux inside the team OPIS (Optimisation, imagerie et santé) at Inria Saclay and CentraleSupélec-Université Paris-Saclay. Since the rise of the COVID19 pandemic, this team worked in developing several tools using deep-learning methods to help in **evaluating the severity of patients infected by the virus.** Proposed in June 2020 in the field of the GENCI COVID19 fast track call the **AI-Severity** tool (project ScanCovIA in partnership with 2 hospitals - Institut Gustave Roussy and Kremlin Bicêtre - and the Owkin startup) aims to **anticipate since the first visit of the patient, if this patient will develop or not a severe form of infection.** Trained using the Jean Zay supercomputer, this tool has been open sourced and now used in production by the 2 hospitals.

MORE INFO

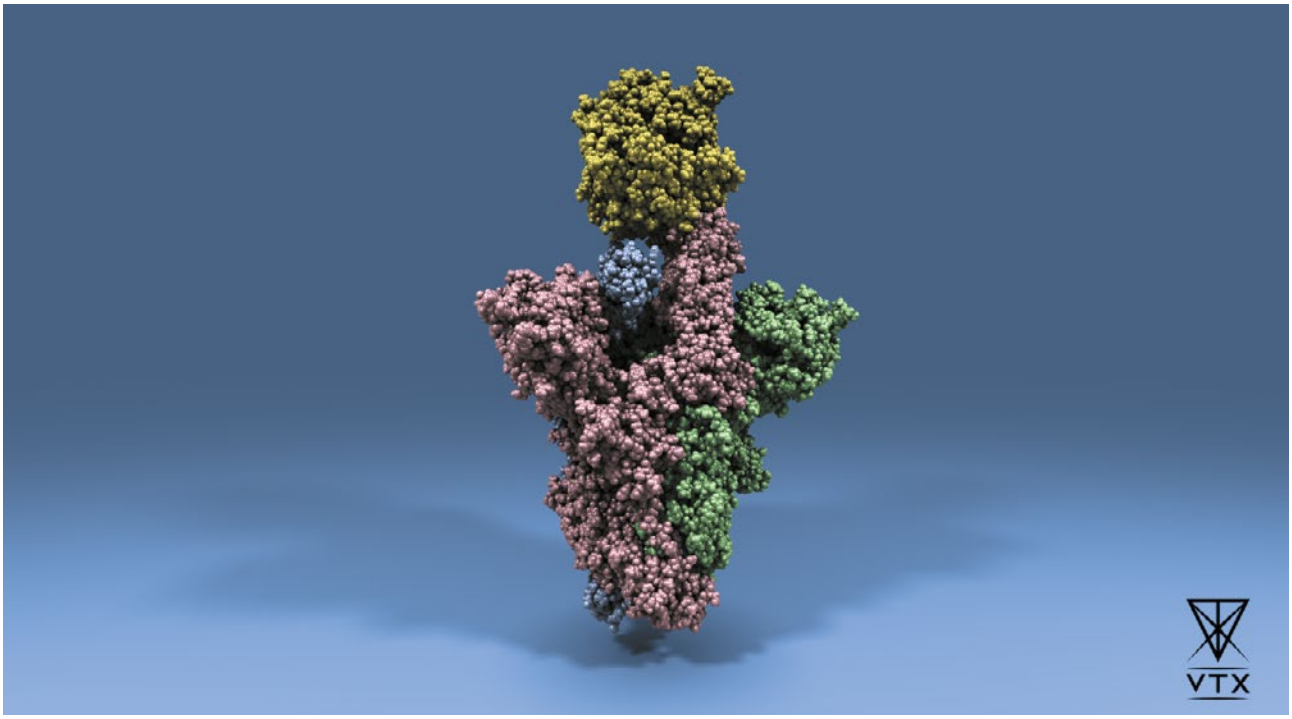
www.nature.com

The partner team at the Gustave Roussy Institute

THE MEANS OF GENCI FACING THE COVID-19

In 2021, facing health emergency, GENCI and the three national centers continued to support scientific research dedicated to fighting against COVID-19. Since the start of the pandemic, nearly 60 projects from academic and industrial research teams, in health, have benefited from the digital power of GENCI thanks to computing resources at national and European levels (PRACE).

Among various aspects studied, we find: the modeling of virus entry into the human body thanks to the study of molecular dynamics between the SARS-CoV-2 Spike protein and the ACE2 protein present on the surface of host cells; the study of the delta variant; the search for ligands that can inhibit the interaction between the virus and the host cell; the screening of existing molecules in large databases to identify possible drugs; the modeling of the transmission of the virus in the air by the transport of pathogens contained in the droplets of saliva emitted during breathing, speaking, coughing, etc.; the analysis of the virus reproduction rate R_0, an indicator allowing to follow its circulation within the population; the simulation of the management of COVID-19 infections in nursing homes and the exploration of Twitter feeds for the analysis of COVID-19 socio-economic impact in France. A document will be produced in 2022 to summarize the research that has been carried out on GENCI's resources.

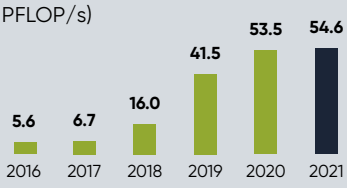


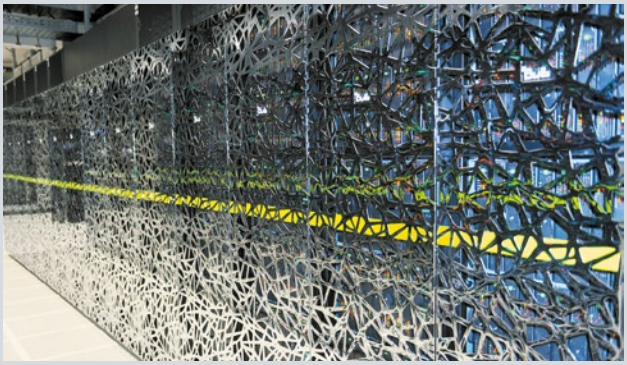
Representation of the interaction between the Spike protein and the ACE-2 receptor (in yellow) visualized with VTX. Data from HPC simulations performed in the framework of the PRACE COVID-HP project.

SERVICES OFFERED BY GENCI

SUPERCOMPUTERS EVOLVE

GROWTH IN COMPUTING CAPACITY
(IN PFLOP/s)





OCCIGEN

ATOS BULLX SUPERCOMPUTER, **3.5 PFLOP/s**

CINES hosts a supercomputer from manufacturer Atos, with a peak power of 3.5 PFLOP/s. Composed of **3,366 nodes** for a total of **85,824 cores** with **Haswell and Broadwell partitions.**

OUTLOOK: From mid-2022, Occigen supercomputer will be replaced by Adastra converged supercomputer, HPE Cray EX4000, with a peak power of more than 70 PFLOP/s, more than 120,000 AMD Genoa cores and more than 1,300 AMD MI250X GPUs.

JEAN ZAY

HPE SGI 8600 SUPERCOMPUTER, **28.3 PFLOP/s**

IDRIS hosts a supercomputer from manufacturer HPE, with a peak power of 28 PFLOP/s composed of a scalar partition and a converged partition with **86,648 CPU cores** and **2,736 V100 or A100 GPUs.**

A **4.9 PFLOP/s** scalar partition based on **1528 nodes** with Intel Cascade Lake processors.

An accelerated partition with a peak power of **23.4 PFLOP/s** based on **650 accelerated nodes** and with **3 A100, 2,712 V100 and 24 A100.**

OUTLOOK: From the beginning of 2022, the supercomputer will be completed by a converged partition of **8.1 PFLOP/s, 52 nodes AMD Rome** octo GPU Nvidia A100, **3,328 cores** and **416 A100.**

JOLIOT-CURIE

ATOS SEQUANA X1000/XH2000 SUPERCOMPUTER, **23 PFLOP/s**

TGCC hosts a supercomputer from manufacturer Atos, with a peak power of 23 PFLOP/s, composed of **4 partitions** including 3 scalar partitions and a partition for pre/post processing based on NVIDIA GPUs.

A first scalar partition of **2,292 AMD Rome nodes,** 12.2 PFLOP/s and **293,376 cores.**

A second scalar partition of **1,656 Intel nodes** based on Skylake, 6.9 PFLOP/s and **79,488 cores.**

A third scalar partition of **828 Intel nodes** based on Knights Landing, 2.2 PFLOP/s and **52,992 cores.**

A fourth accelerated partition of **32 NVIDIA nodes** based on V100, 1.2 PFLOP/s and **128 GPUs.**

A fifth prototype partition of **3,648 cores** based on Fujitsu ARM A64FX processors, 0.3 PFLOP/s

NEOWISE

AMD PROTOTYPE: AMD GLOBAL DONATION PLAN TO FIGHT AGAINST COVID-19

The Grid'5000 site of ENS Lyon hosts an accelerated partition of **480 AMD Rome cores** and **80 MI50, 0.5 PFLOP/s.**

ACCESS MODALITIES TO GENCI'S NATIONAL RESOURCES

DARI PORTAL

www.edari.fr

National computing and storage resources are made available free of charge for high performance computing and Artificial Intelligence (AI) scientific projects, from academic and industrial spheres. To be eligible, open research work must be submitted for publication at the end of the allocation period. Any computing resources request must be submitted as part of a call for projects via www.edari.fr portal, common for the three national computing centers (CINES, IDRIS and TGCC). In 2021, three types of access allowed to obtain resources depending on user needs: preparatory access, regular access and dynamic access. Following the success of dynamic access initially intended for the AI community on Jean Zay at IDRIS, we worked in 2021 to extend this type of access to all Thematic Committees (TC) and to all machines in national centers. Since January 10, 2022, it is now possible to apply at any time, for each TC, via a single form, for dynamic access (requests ≤ 50,000 GPU hours / 500,000 CPU hours) or regular access if requests are more important. It is no longer possible to apply to a preparatory access, code optimization can now be performed with a dynamic access. Expertise and allocation periods remain unchanged for regular access.

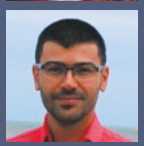
ACCESS MODALITIES

2021	2022
TYPE OF ACCESS AND NEEDS	
PREPARATORY ACCESS Code optimization	
REGULAR ACCESS (RA) High performance computing and use of Artificial Intelligence (AI)	**REGULAR ACCESS (RA)** High performance computing and AI **Request > 50,000 GPU hours/ 500,000 CPU hours**
DYNAMIC ACCESS (DA) Development of AI algorithms and methodologies, use of AI	**DYNAMIC ACCESS (DA)** High performance computing and AI Code optimization **Request ≤ 50,000 GPU hours/ 500,000 CPU hours**
TO APPLY	
3 FORMS TO FILL OUT → 3 TYPES OF ACCESS	**A SINGLE FORM TO FILL OUT → REDIRECTION TO RA OR DA**
PROJECT LEADERS AND THEMATIC COMMITTEES	
• **RA:** all Thematic Committees • **DA:** CT10 dedicated to AI	**RA and DA:** all Thematic Committees
NATIONAL RESOURCES AVAILABLE	
• **RA:** production supercomputers at CINES, IDRIS and TGCC • **DA:** AI partition at IDRIS	**RA and DA:** production supercomputers at CINES, IDRIS and TGCC
SERVICES AVAILABLE FOR ANY TYPE OF ACCESS	
• DATA VISUALIZATION AND PROCESSING • USER SUPPORT AND CENTER SUPPORT	

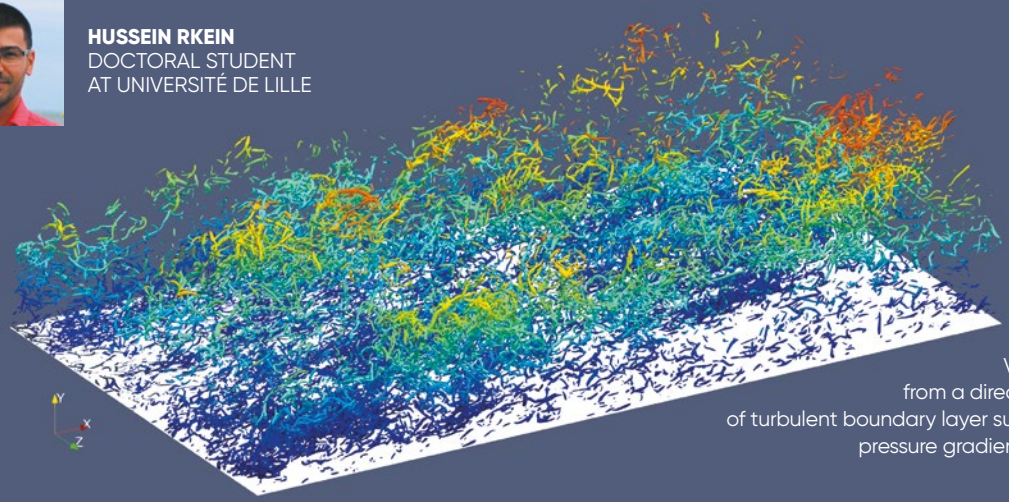
SOME EXAMPLES OF SIMULATIONS

These numerical simulations were carried out within the framework of the thesis of Hussein RKEIN. The objective is to build a very detailed database for the study of the turbulence properties in the vicinity of a wall. The parameters of the simulation have been chosen so that the flow is representative of a flow on a small part of an aircraft wing. This database should allow a better understanding of the turbulence and propose improvements on the models which do not give complete satisfaction for this type of flow in the presence of a pressure gradient.

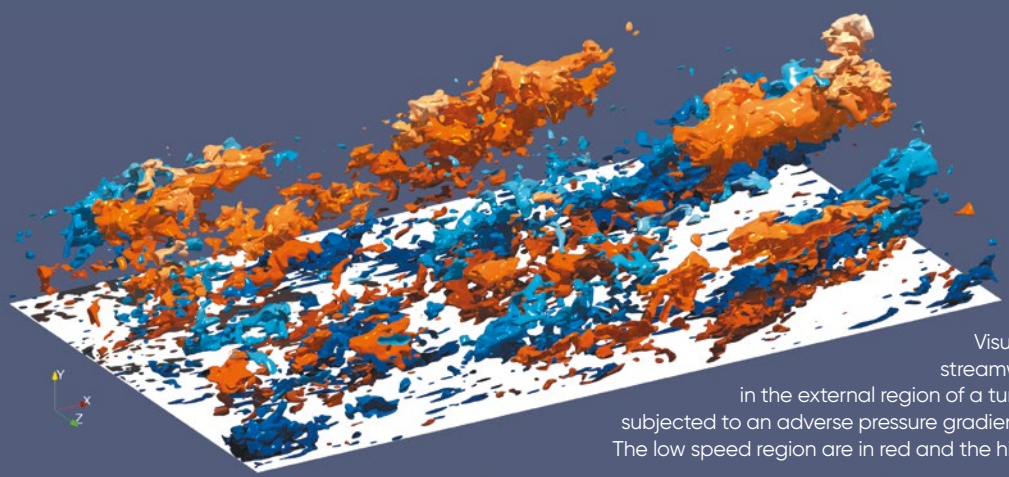
JEAN-PHILIPPE LAVAL
CNRS RESEARCH DIRECTOR
AT "LABORATOIRE DE MÉCANIQUE DES FLUIDES DE LILLE - KAMPÉ DE FÉRIET".



HUSSEIN RKEIN
DOCTORAL STUDENT
AT UNIVERSITÉ DE LILLE



Visualization of vortices from a direct numerical simulation of turbulent boundary layer subjected to an adverse pressure gradient (6,800 < Reθ < 7,600).
J.-P. Laval & H. Rkein, LMFL



Visualization of fluctuating streamwise velocity structures in the external region of a turbulent boundary layer subjected to an adverse pressure gradient (6,800 < Reθ < 7,600). The low speed region are in red and the high speed ones in blue.
J.-P. Laval & H. Rkein, LMFL

FOREWORD BY THE CHAIR OF GENCI'S EVALUATION COMMITTEE

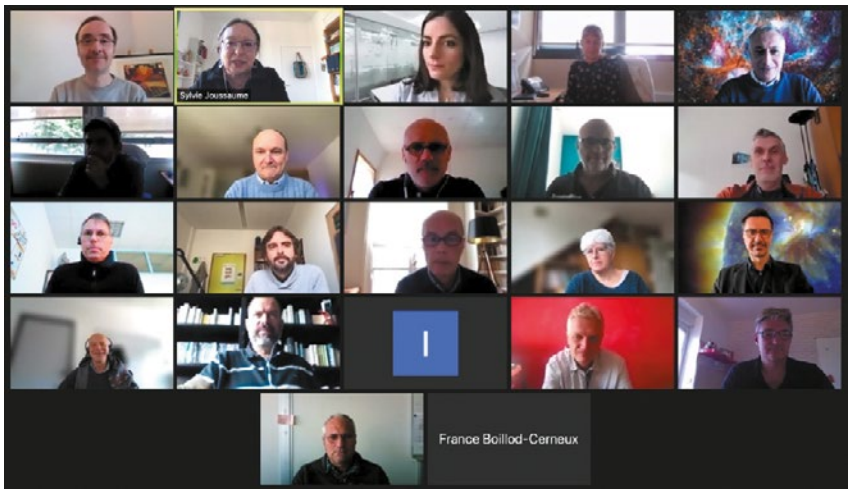
BY SYLVIE JOUSSAUME, CHAIR OF GENCI'S EVALUATION COMMITTEE

2021 has been marked by a continued significant pressure on high-performance computing resources. However, the greater availability of computing resources at the national level, following the reduction in the hours dedicated to PRACE, and the possibilities of transferring applications between machines, have made it possible to optimize these pressures during the DARI A10 and A11 allocations. In particular, this made it possible to compensate for the temporary break of allocations to CINES for A11, pending the commissioning of the new Adastra machine next spring. This increased availability also enabled a special major challenge session for 20 projects on A10.

The year 2021 was also devoted to the preparation of the exascale project for France. Many of you were involved in the working group to present an overview of the main computing codes of the French scientific community and to explain their future needs, in particular in support to prepare for accelerated architectures, a challenge for many communities.

The year 2022 will be a year of change, with not only the arrival of a new machine but also the implementation of the expansion of dynamic access for small projects, in which the chairs of the thematic committees have been associated.

> // The year 2022 will be a year of change, with not only the arrival of a new machine but also the implementation of the expansion of dynamic access for small projects. //



Evaluation Committee Meeting A11, October 7, 2021.

FOREWORDS BY THE CHAIRS OF THE THEMATIC COMMITTEES

CT1
ENVIRONMENT
GERHARD KRINNER
Chair of CT1

The projects submitted to TC1 are very diverse in terms of themes, volume, and approaches. Climate modeling is predominant in terms of the number of projects and the resources requested. The fair and balanced evaluation of projects of very different sizes - the resources required can vary by a factor of more than 1,000 between projects - is a particular point of attention. The planned evolution of GENCI's access to resources may resolve some of the difficulties associated with this diversity.

CT2A
NON REACTIVE AND MULTIPHASE FLOWS
GUILLAUME BALARAC
Chair of CT2a

The simulation of flows covers a wide range of activities, from fundamental analysis to technology transfers. The 65 projects of this year show this diversity, by increasing our understanding of turbulent flows and of the associated hydrodynamic instabilities existing in applications at the heart of today's key challenges: energy, environment, processes, transport, health…

CT2B
REACTIVE AND MULTIPHASE FLOWS
PASCALE DOMINGO
Chair of CT2b

In 2021, 42 projects submitted to CT2b have received CPU time on the supercomputers from GENCI, among these projects around 10 were new projects. Some projects have been hampered by the COVID crisis, essentially because the planned recruitment of foreign PhD students and post-doc researchers has been canceled or delayed.
The research topics covered by CT2b are extremely varied since all aspect of reactive and/or multiphase fluids mechanics are covered. Transition towards decarbonated energy is present through projects covering hydrogen use or solar energy.
The great majority of the softwares used and developed in this community presents good performances on the panel of computers proposed by GENCI, which facilitate the attribution process.

CT3
BIOLOGY AND HEALTH
LAURENT DESBAT
Chair of CT3

The "CT3" (biology and health) evaluated 8 projects (+4 additional requests) in A10 and 8 in A11, including 4 new projects, for a global allocated computing time (in Mh): Jean Zay CPU 13.3 et GPU 0.6, Occigen 2.5, Joliot Curie SKL 10, Rome 26.5. The projects concern usual scientific fields: genetics, molecular dynamics, fluid dynamics, biomechanics, medical imaging, etc.

CT4
GEOPHYSICS AND ASTROPHYSICS
GEOFFROY LESUR
Chair of CT4

In 2021, the CT4 panel has reviewed 65 proposals, similarly to previous years. The proposals were excellent and very diverse. The largest proposals were focusing on stellar formation, dynamos and cosmology. We also observe a strong growth a proposals targetting GPU architectures (+500%), as a result of new codes developped in the community, which are now being used in large-scale production runs.

CT5
THEORETICAL PHYSICS AND PLASMA PHYSICS
ÉRIC SERRE
Chair of CT5

In 2021, 30 very high-quality projects have used 500 million of computing hours to cover a broad spectrum of applied and fundamental researches. Although the number of project is decreasing, partly due to the pooling of numerical codes, the number of hours is rising sharply to reach around 25% of the total resource. It is the QCD needs that have led to this very strong increase.

CT6
COMPUTING, ALGORITHMS AND MATHEMATICS
DIDIER AUROUX
Chair of CT6

In the continuity of previous years, CT6 evaluated 16 projects in 2021, including 2 submitted by companies. They cover a wide range of topics from numerical algorithms to parallelization problems (resolution of large linear systems, development of libraries, scalability). The majority of projects are motivated by applications from other disciplines: physics, biology, medicine.

CT7
MOLECULAR MODELLING APPLIED TO BIOLOGY
PATRICK FUCHS
Chair of CT7

In 2021, the CT7 assessed 30 to 40 requests per call, for a total of CPU hours of 60-80 million and 2-3 million GPU hours. The trend is confirmed with the net increase in demand for GPUs thanks to a successful code porting. However, the demand for CPU is also increasing. Most of the projects concern molecular dynamics of proteins in their lipid or aqueous environment. The size of the studied systems often reaches several million atoms. Thus, the resources of GENCI and the competence of the centers are decisive in carrying out these studies.

CT8
QUANTUM CHEMISTRY AND MOLECULAR MODELLING
DAVID LOFFREDA
Chair of CT8

During the year 2021, theoretical modeling in quantum chemistry has advanced in the knowledge of chemical bonding, keeping its many fields of application and working on two fronts: the development of quantum codes and their use. Their performance and robustness now allow the development of realistic models of organic, organometallic, catalytic, electrochemical and biological systems. This year resulted in a further increase in the required computational resources, in a context where a permanent access to them was decisive. The current developments open a promising route towards the transferability of these codes on the machines of new generation. These benefit from the technical support of the three GENCI centers, which the committee thanks for their support.

CT9
PHYSICS, CHEMISTRY AND MATERIALS PROPERTIES
THIERRY DEUTSCH
Chair of CT9

The number of files is constant compared to last year at about 110 requests for allowances with a rate of new files of about 20%. The average number of requests for hours is one million two hundred thousand hours and is constantly increasing. Neural network learning has established itself as a new solution in materials simulation.
This year saw the emergence of priority research programs and equipment (PEPR), particularly in the field of materials with the PEPR Diadème, which focuses on digital technology to accelerate the discovery of new materials. This PEPR should offer new services to users and allow the democratization of simulation but also advanced data analysis solutions for the experimental community. The appearance of dynamic access for projects of less than 500,000 hours should also facilitate access to national computing resources.
Nevertheless, there remains the problem of training in these new tools, particularly in scripting languages such as Python, in good programming practices, and of course in data management.

CT10
NEW APPLICATIONS AND MULTIDISCIPLINARY APPLICATIONS OF HPC
BRUNO SCHEURER
Chair of CT10

Despite the pandemy, 2021 has seen a growth for the number of proposals (18) and for the allocation (100 Mh CPU and 10 Mh GPU).
Artificial Intelligence (AI) is now the main source of proposals (15) aside planet mineralogy, nuclear reactors and electromagnetism. IA proposals are studying neural networks for many fields of research. One may quote robotics and autonomous agents, natural language processing, image and videos analysis, model reduction for numerical simulation.

2021 • MAIN SCIENTIFIC RESULTS

The scientific results described in the following pages are the fruits of research work during 2021 using the computing resources of GENCI.

Whilst these projects are representative of the range of scientific fields using the national supercomputers, they are but a snapshot of the 1,157 projects that were allocated computing time in 2021.

MORE RESULTS ON OUR WEBSITE

www.genci.fr

CT5 THEORETICAL PHYSICS AND PLASMA PHYSICS **JEAN ZAY: 5 MILLION HOURS - JOLIOT-CURIE: 22 MILLION HOURS**

DANIELE DEL SARTO,
ASSISTANCE PROFESSOR, INSTITUT JEAN LAMOUR, UMR 7198, UNIVERSITÉ DE LORRAINE

ERWAN DERIAZ,
RESEARCHER, INSTITUT JEAN LAMOUR UMR 7198, CNRS

ETIENNE GRAVIER,
PROFESSOR, INSTITUT JEAN LAMOUR UMR 7198, UNIVERSITÉ DE LORRAINE

MAXIME LESUR,
ASSISTANT PROFESSOR, INSTITUT JEAN LAMOUR, UMR 7198, UNIVERSITÉ DE LORRAINE

THIERRY RÉVEILLÉ,
ASSISTANT PROFESSOR, INSTITUT JEAN LAMOUR, UMR 7198, UNIVERSITÉ DE LORRAINE

ALAIN GHIZZO,
PROFESSOR, INSTITUT JEAN LAMOUR UMR 7198, UNIVERSITÉ DE LORRAINE

THEORETICAL PHYSICS

Semi-Lagrangian and multi-scale simulations of the Vlasov equation for the modeling of hot plasmas

The central theme of the team is modeling and numerical experimentation in plasma physics where kinetic and microscopic effects are dominant, in particular in magnetic field generation due to anisotropy of velocity distribution functions (Weibel instability), in their dissipation due to magnetic reconnection, or in the transport of impurities in tokamak plasmas for magnetic confinement fusion research.

This first example concerns the generation of a magnetic field in Weibel-type instability. In Fig. 1, a numerical simulation of the beam-plasma interaction in the relativistic regime is performed on Jean Zay using 2048 cores (allocation of 2Mh), considering a configuration of two electron beams propagating in opposite directions. Such a configuration is unstable and leads to the generation and amplification of an intense magnetic field. Using a semi-Lagrangian (VLasov ElectroMagnetic solver) VLEM [1, 2] code, we have shown a correlation between the entropy violation and the energy transfer (kinetic towards magnetic energy), induced by the microscopic fluctuations of the distribution function. We observe in Fig. 1 a reversible time evolution in the topology of the magnetic field. We could thus highlight the reversible character of this energy transfer [3] in agreement with the information theory and new heating process.

This type of problem also concerns magnetic reconnection where the multi-scale character becomes essential. An MHD AMR code has been developed to deal with the multiscale aspect, in the framework of a GENCI-DARI project *"Nonlinear dynamics of current sheets in magnetic reconnection"* [10-11]. This AMR technique could be adapted to solve the Vlasov-Maxwell system.

This second example concerns the impurities transport in tokamaks. The impurity transport is complex and results from turbulence (anomalous transport) and collisions on the main ion species (neoclassical transport). Both channels may not be additive and exhibit synergistic properties, as recently highlighted [4].

The code is currently developed in IRFM-CEA and is named GYSELA-5D (GYrokinetic Semi-Lagrangian [6]). From a theoretical point of view and using the results of the nonlinear simulations, the different terms involved in transport (diffusion, pinch speeds, neoclassical and turbulent contributions, etc.) have been highlighted especially thanks to the neoclassical and quasi-linear theories [7-8] (see Fig. 2).

Moreover, a newly implemented vorticity source that polarizes the system allows an ExB velocity shear and a transport barrier and a pedestal to be triggered (High-confinement mode). For sufficiently large shearing rates, turbulent transport is suppressed, and a transport barrier builds up. These results have been compared with those given without transport barrier [8], and the transport barrier is proven efficient in reducing the magnitude of turbulent plasmas [9].

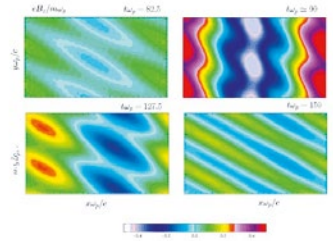


Fig. 1 : Contours of the (normalized) magnetic field component Bz at four different times for a simulation, performed with the VLEM code, of the excitation of a broad spectrum of oblique filamentation modes. After saturation of the instability (top left frame), the energy transfer is reversed.

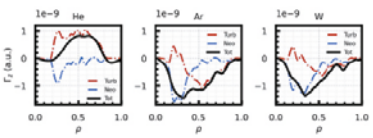


Fig. 2 : Impurity fluxes for different impurities (numerical simulations performed with GYSELA). The total impurity flux (black solid line) is divided into a turbulent part (red dashed line) and a neoclassical part (blue dashed line).

These investigations correspond to the PhD programs of Kyungtak Lim and Guillaume Lo-Cascio, which involve both Lorraine University and IRFM-CEA teams.

TERESA simulations [7] have been performed on Jean Zay-IDRIS for a total of 5 million core.hours. GYSELA simulations [8-9] have been performed on IRENE-TGCC for a total of 22 million core.hours. This work is part of a Eurofusion project (TSVV#6).

[1] E. Sonnendrücker, J. R. Roche, P. Bertrand, A. Ghizzo, J. Comput. Physics 149, 201 (1999). [2] M. Sarrat, A. Ghizzo, D. Del Sarto, L. Serrat, Eur. Phys. J. D 71,271 (2017). [3] A. Ghizzo and D. Del Sarto, Plasma Phys. Control. Fusion 63, 055007 (2021). [4] P. Donnel et al., Phys. Plasma Control. Fusion, 61, 044006 (2019). [5] T. Drouot et al., Phys. Plasmas 22, 082302 (2015). [6] V. Grandgirard et al., Comput. Phys. Communications, 207, 35 (2016). [7] K. Lim et al., Plasma Phys. Cont. Fusion 62, 095018 (2020). [8] K. Lim et al., Nucl. Fusion 61, 046037 (2021). [9] G. Lo-Cascio et al., in progress (2022). [10] D. Del Sarto, E. Deriaz, J. Comput. Phys. 351, 511 (2017). [11] H. Betar, D. Del Sarto, M. Ottaviani, A. Ghizzo, Phys. Plasmas, 27, 102106 (2020)

CT1 ENVIRONMENT **OCCIGEN: 250,000 HOURS**



BENOÎT URRUTY,
DOCTORAL STUDENT, UNIVERSITÉ GRENOBLE ALPES
FABIEN GILLET-CHAULET,
RESEARCHER, UNIVERSITÉ GRENOBLE ALPES
OLIVIER GAGLIARDINI,
PROFESSOR, UNIVERSITÉ GRENOBLE ALPES

Institut des Géosciences de L'Environnement (Univ. Grenoble Alpes, CNRS, IRD, INP)

EARTH AND UNIVERSE SCIENCES

Tipping points of the Antarctic Ice-Sheet

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The polar ice caps are important components of the climate system. A volume of ice representing a 58 m change in sea level elevation is stored on the Antarctic continent. The ice, which forms from the accumulation of snowfall, behaves like a viscous fluid that flows under its own weight. The Antarctic ice cap is unique in that it rests on a bedrock with large areas below sea level and is surrounded by large ice shelves which, due to water pressure, float on the oceans. This particular configuration is subject to instability where a small disturbance, such as increased melting under the floating shelves, could lead to a significant and irreversible retreat of the ice sheet. Recent observations have shown a significant acceleration of some of the glaciers draining the ice-sheet, particularly in the Amundsen Sea area, suggesting that this mechanism may have been initiated.

IGE has been co-developing the Elmer/Ice ice-sheet model for several years. It is mainly the initial and boundary conditions that cause difficulties. For example, the conditions at the base are inaccessible to measurement, yet the resistance of the base to ice sliding can vary over several orders of magnitude depending on the type of substrate and the presence of liquid water. The result is an extremely heterogeneous flow where the majority of the ice is drained by outflow glaciers, true rivers of ice within the ice-sheet, which can flow at a rate of a few kilometres per year as illustrated in the Figure. An adaptive mesh and data assimilation methods allow us to capture the flow velocities observed by satellites. Thanks to GENCI resources, we have shown with our partners in the European TiPACCS project that the ice-sheet is currently in a stable configuration in the face of small perturbations.

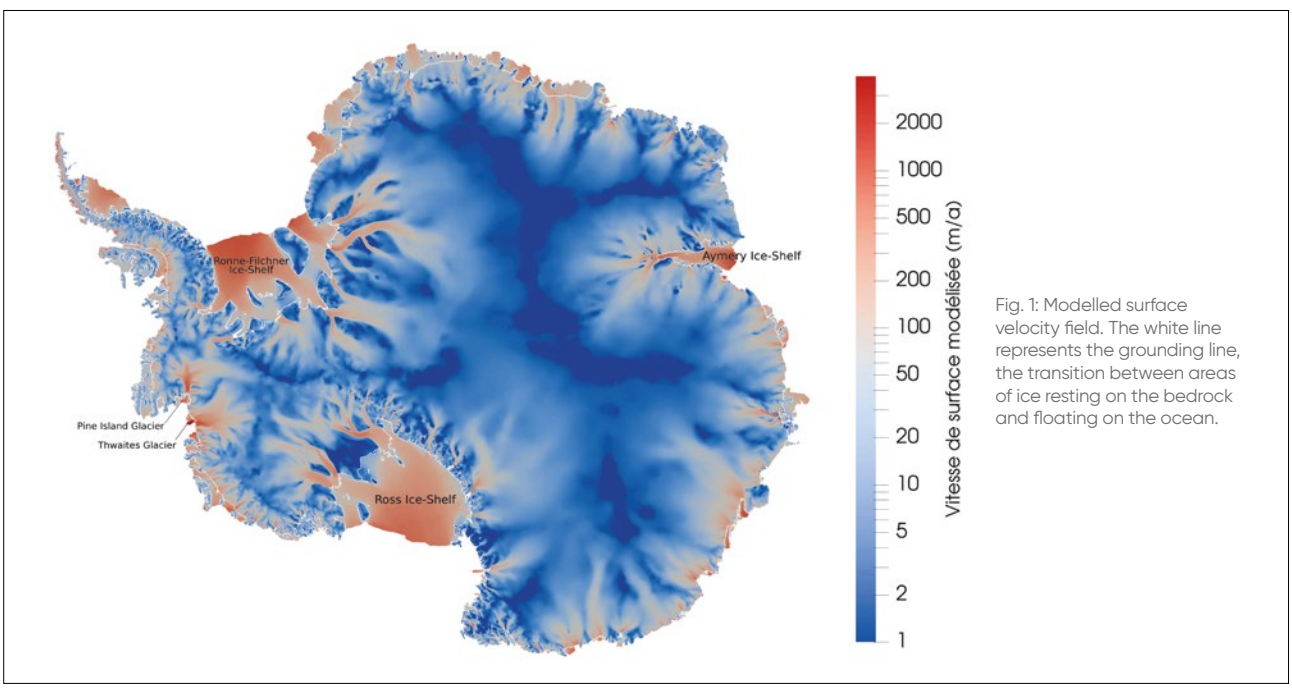


Fig. 1: Modelled surface velocity field. The white line represents the grounding line, the transition between areas of ice resting on the bedrock and floating on the ocean.

CT4 GEOPHYSICS AND ASTROPHYSICS **JEAN ZAY: 1.2 MILLION HOURS - JOLIOT-CURIE ROME: 2 MILLION HOURS**

JÉRÉMY FENSCH,
ASSISTANT PROFESSOR
ECOLE NORMALE SUPÉRIEURE DE LYON

Centre de Recherche Astrophysique de Lyon

EARTH AND UNIVERSE SCIENCES

Turbulence in primordial galaxies

Primordial galaxies are very different from local ones. Disks of the former are not composed of spiral arms, but of giant clumps which form stars in a vigorous way and are very turbulent. And it is this turbulence which generate supersonic motions able to strongly compress the gas, triggering its gravitational collapse and thus its conversion into stars.

The origin of this turbulence is still debated: is it generated by galactic dynamics or by young stars, via their ionizing radiation of supernovae explosions? Yet, local dynamics depend upon global morphology and young stars would not have the same effect if they are located in clumps or spread along spiral arms. Both processes are thus very likely to differ between galaxies of the young or recent Universe.

The purpose of my work is to understand how this turbulence is generated and what is its effect on star formation in galactic disks during their cosmic history. To this aim, one needs to model the interaction between, on the one hand the global galactic dynamics and star formation and on the other hand the galactic gas. The numerical challenge arises from the spatial dynamical range playing a role, and the associated memory cost.

To do so, I have used the GENCI resources to develop a zoom method inside a clumpy disk. This way, global dynamics is captured along with star formation at the highest resolution of 0.38 pc (see Fig.1). In order to differentiate the effect from dynamics and stars, I have cut to ionizing radiation and supernovae explosions. According to preliminary studies, the turbulent energy only decreases by around 20%, implying a dominance of dynamical effects over stellar effects.

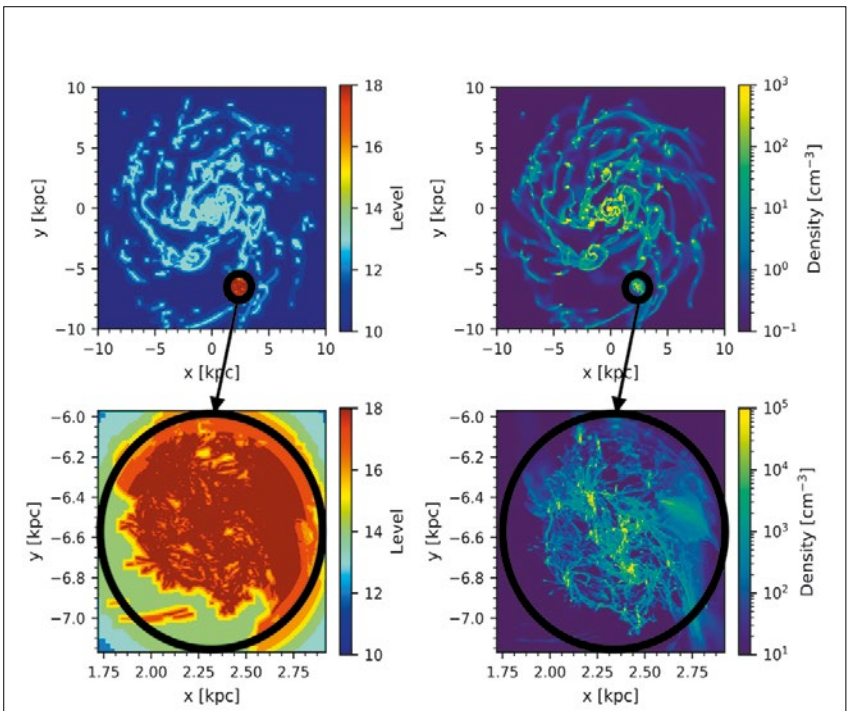


Fig.1: Refinement level and density maps of the zoomed giant clump in one of the simulations.

CT2A NON REACTIVE AND MULTIPHASE FLOWS **OCCIGEN: 10 MILLION HOURS - JOLIOT-CURIE: 8 MILLION HOURS**



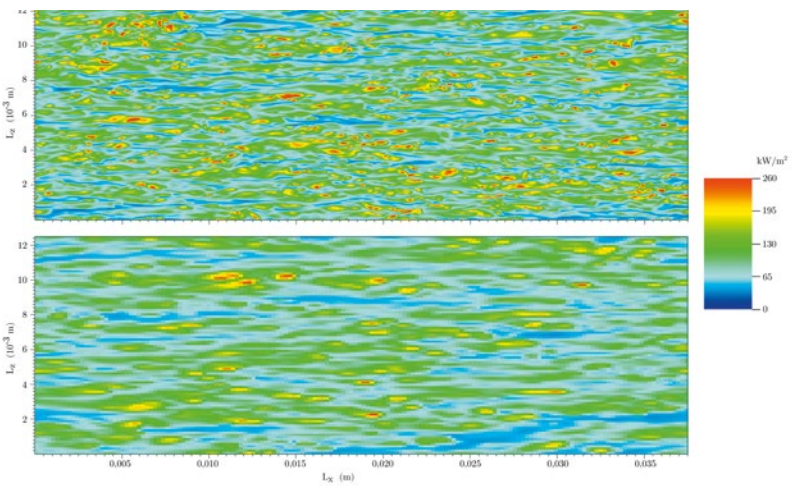
MARTIN DAVID,
TEMPORARY TEACHING AND RESEARCH ASSISTANT (ATER)
ADRIEN TOUTANT,
RESPONSIBLE FOR SOLAR POWER PLANTS IN THE NEXT GENERATIONS (CSPG)
FRANÇOISE BATAILLE,
DIRECTOR OF THE PROMES LABORATORY

Laboratoire PROMES-CNRS (UPR 8521), Université de Perpignan via Domitia

FLUID MECHANICS

Multi-scale approach for solar receivers: from the physics of temperature/turbulence couplings to the correlation development

Numerical simulations have been carried out for research on the new generation of concentrated solar power plants. The numerical resolution of the coupled Navier-Stokes and internal energy equations in a plane channel gives the ability to perform fundamental studies of the flow in gas-pressurized solar receivers. These flows are very complex since they are highly turbulent and asymmetrically heated. Characterized by very high temperatures reaching 1,000 °C, they are the place of intense heat transfers and strong couplings between dynamics and temperature. The developed multi-scale approach improved the flow knowledge by filling gaps of the literature at each level and provided turbulence models that will facilitate the industrial soaring of new tower power plants.



Simulation performed by Martin David during his thesis, supervised by Adrien Toutant and Francoise Bataille, during the DARI GENCI 2020-A0082A05099 grant.

Fig. 1: Instantaneous conductive flow fields at the hot wall (1000°C) for a Reynolds number of 70000. On the top, the results of a direct numerical simulation are shown; on the bottom, those of a large-scale turbulence simulation.

The detailed levels of study feed the more macroscopic levels. At the local scale, Direct Numerical Simulations (DNS) are performed to deepen the knowledge of the interactions between turbulence and temperature [1] (unit cost: 4 million of computational hours). At the intermediate scale, Large Eddy Simulations (LES) are achieved on coarser grids which leads to a significant reduction of the computational costs (12000 hours). The goal is to develop subgrid-scale models that reproduce the effect of the small structures on the resolved scales. Tests are carried out by comparing the results of each LES with those of DNS [2] (see figure). Thanks to these assessments, we identify an accurate and reliable model. This latter was used to perform 70 LES to develop a correlation that estimates the heat transfers in asymmetrically heated channels [3]. This constitutes a study at a macroscopic level since the correlation could be used to conduct investigations at the solar receiver scale [4].

[1] M. David, A. Toutant, et F. Bataille, « Direct simulations and subgrid modeling of turbulent channel flows asymmetrically heated from both walls », Phys. Fluids, vol. 33, no 8, 2021. [2] M. David, A. Toutant, et F. Bataille, « Investigation of thermal large-eddy simulation approaches in a highly turbulent channel flow submitted to strong asymmetric heating », Phys. Fluids, vol. 33, no 4, p. 045104, 2021. [3] M. David, A. Toutant, et F. Bataille, « Numerical development of heat transfer correlation in asymmetrically heated turbulent channel flow », Int. J. Heat Mass Transf., vol. 164, p. 120599, 2021. [4] M. David, A. Toutant, et F. Bataille, « Impact of asymmetrical heating on the uncertainty propagation of flow parameters on wall heat transfers in solar receivers », Appl. Therm. Eng., vol. 199, p. 117547, 2021.

CT2B REACTIVE AND MULTIPHASE FLOWS **OCCIGEN & JEAN ZAY: 3.8 MILLION HOURS**



FLORIAN LE ROY DE BONNEVILLE,
DOCTORAL STUDENT AT TOULOUSE INPT, INSTITUT DE MÉCANIQUE DES FLUIDES DE TOULOUSE
RÉMI ZAMANSKY,
ASSISTANT PROFESSOR, INSTITUT DE MÉCANIQUE DES FLUIDES DE TOULOUSE
FRÉDÉRIC RISSO,
CNRS RESEARCH DIRECTOR, INSTITUT DE MÉCANIQUE DES FLUIDES DE TOULOUSE

Institut de mécanique des fluides de Toulouse, CNRS/Université Paul Sabatier/ Institut National Polytechnique de Toulouse

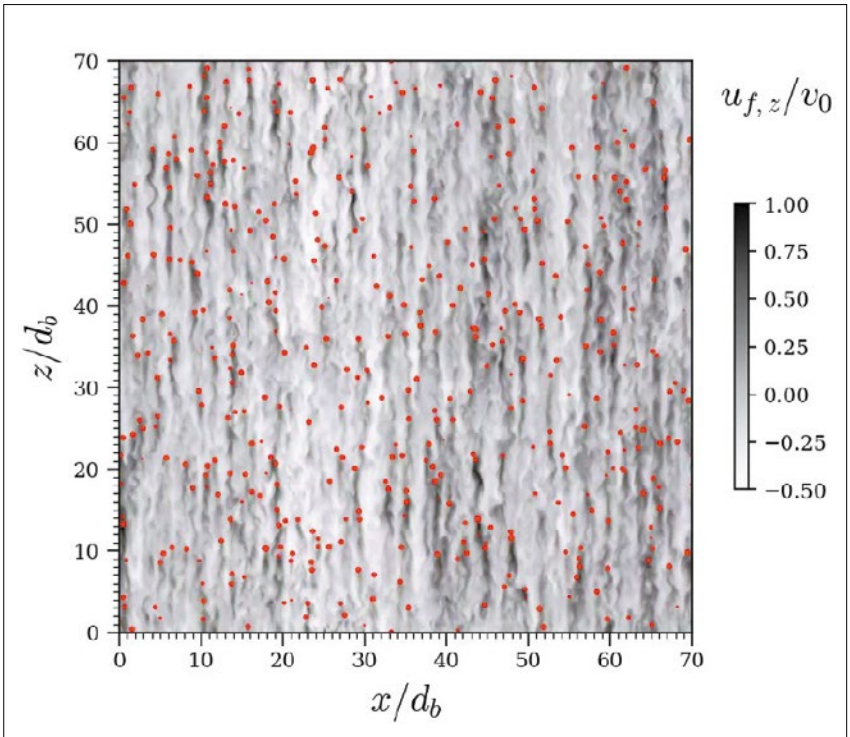
FLUID MECHANICS

Turbulence induced by a bubble swarm

Bubble flows are encountered in many natural phenomena, industrial processes, or accidental situations, such as in certain scenarios of core meltdown in a nuclear power plant.

Because of their low density, the bubbles are set in motion by Archimedes' force and the rise of the bubbles drives the fluid. It is a complex system in which the bubbles and the liquid are coupled, leading to the emergence of collective phenomena and original properties of the flow. Several parameters influence these mechanisms: the number of bubbles, their size, their speed, the liquid viscosity, etc. We study the rise of a swarm of bubbles of sufficient size to produce large wakes, so that the flow is driven by the interactions between these wakes. From an application point of view, this type of flow is characterized by intense agitation favoring transfers between phases and mixing.

Although the equations describing precisely this type of flow are relatively well known, their numerical simulation remains out of reach, due to the large spectrum of temporal and spatial scales involved. In order to simulate these flows and to understand the turbulent transfer and the mixing mechanisms, we simplify these models by neglecting the precise description of the interfacial dynamics. This allows us to simulate flows with a large number of bubbles and to emphasize the interactions between wakes. The main difficulty with this type of calculation comes from the fictitious self-interaction of a bubble with its own wake. We have established a method to correct this effect and to accurately calculate the trajectory of each bubble. Our allocation on the Occigen and Jean Zay machines allowed us to obtain numerical simulations of the turbulence induced by a swarm of bubbles in agreement with the experiment, as illustrated opposite.



Instantaneous field of the vertical velocity of the liquid. The circles materialize the bubbles.

CT9 PHYSICS, CHEMISTRY AND MATERIALS PROPERTIES | **JOLIOT-CURIE & OCCIGEN: 6.2 MILLION HOURS**

NATHALIE VAST, CEA RESEARCH DIRECTOR

From left to right and top to bottom: **Raja Sen** (IPP postdoctoral Researcher), **Jelena Sjakste** (CNRS Researcher), **Amrita Chakraborti** (Postdoctoral Researcher at Bayreuth University - Germany), **Yeonsoo Cho** (IPP Ph.D. Student), **Antoine Jay** (Postdoctoral Researcher at LAAS, CNRS, Toulouse), **Olivier Hardouin Duparc** (CNRS Researcher)

The Materials Science Theory team of the Laboratory of Studies of Irradiated solids, Institut Polytechnique de Paris (IPP) , CEA-DRF-IRAMIS, CNRS UMR 7642

BIOLOGY, CHEMISTRY AND MATERIALS

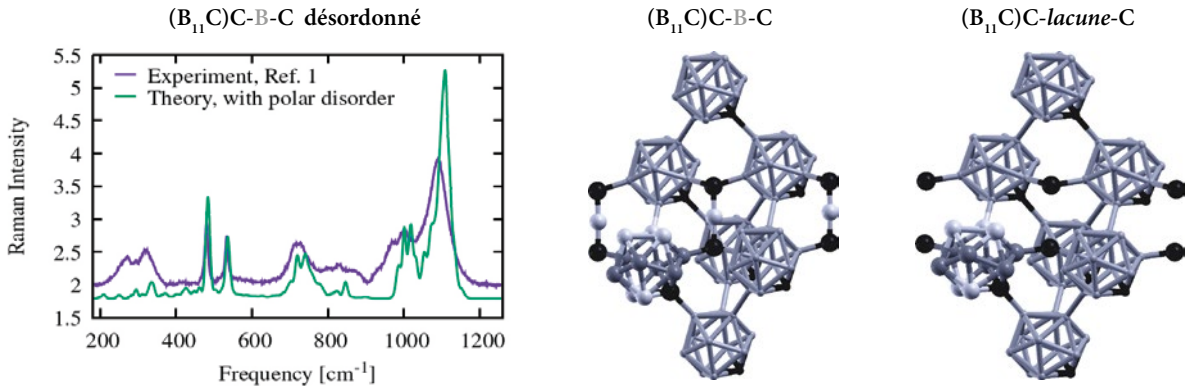
Predicting the physical properties of materials

Our field of research is theoretical and numerical physics for materials science, and consists in the *ab initio* study of physical properties of materials, mainly with quantum-scaled methods based on the density functional theory (DFT). The latter enables us to reduce the complexity of the Schrödinger equation by using the theorem according to which the properties of the electronic ground state of a system of atoms and their electrons are determined uniquely by the electronic density of the ground state.

DFT calculations are performed without adjustable parameters, which has made it possible to predict with success and reliability the physical properties of many materials with controllable accuracy. An example is given *(figure on the left)* for B4C boron carbide, one of the hardest ceramics which is used for shielding military equipment and protecting people (bullet-proof vests). B_4C is also an excellent neutron absorber useful for controlling the chain reaction in future fast neutron reactors.

For this material, we had theoretically predicted that the least energetic vacancy-based point defect is the ejection of the boron B atom from the C-B-C chain *(center figure)*, yielding C-vacancy-C configurations *(right figure)* which weaken the mechanical strength of B_4C. A series of experiments conducted at the Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC, Paris), using the very recent Paris-Edinburgh press with rotating anvil for tomography (RoToPEC), allowed to apply a torsional deformation to boron carbide, driving it in a controlled way into the plastic regime.

The damage have then been analysed by synchrotron X-ray diffraction and Raman spectroscopy, and interpreted using our DFT calculations. New peaks appearing in the two characterization methods turn out to be fingerprints of boron vacancies in the chains, in agreement with the theoretical prediction. This recent result confirms some of the ideas to strengthen B_4C that are actively pursued with our partners from the IMPMC, the Institut de Recherche sur les CERamiques (IRCER, Limoges), and the Institut de Chimie de la Matière Condensée de Bordeaux (ICMCB).



Example of Raman spectrum computed within the density functional theory (left figure) of boron carbide, modelling the substitutional disorder of carbon atoms in polar sites of the B11C icosahedra by a supercell containing 405 atoms (blue line), compared with the experiment (violet line) [Credit: Physical Review Materials, 6 (2022) 016602]. Atomic structure of boron carbide in the ground state (center figure) and after plastic deformation (right figure [Credit: Acta Materialia, 226 (2022) 117553].

CT8 QUANTUM CHEMISTRY AND MOLECULAR MODELLING **OCCIGEN, JEAN ZAY & JOLIOT-CURIE: 4.3 MILLION HOURS**

RICHARD OPOKU, PHD STUDENT, UMR8523

From left to right and top to bottom: **Antoine Roose** (Researcher, UMR8523), **André Severo Pereira Gomes** (CNRS Researcher, UMR8523), **Florent Réal** (Assistant Professor, UMR8523), **Denis Duflot** (Assistant Professor, UMR8523), **Valérie Vallet** (CNRS Research Director, UMR8523), **Céline Toubin** (Professor, UMR8523)

UMR8523, Université de Lille

BIOLOGY, CHEMISTRY AND MATERIALS

Understanding physical and chemical processes in aerosols at the molecular level through multiscale modeling

The term aerosols denotes a suspension of fine solid particles or liquid droplets in air, or another gas. These particles may be natural (e.g. volatile organic compounds emitted by biomass, ice nuclei etc) or man-made (e.g soot from incomplete combustion). An important role played by aerosols is being substrates over which the multitude of gaseous species present in the atmosphere can attach themselves to (and thus carry species, including radionuclides such as iodine, across the globe), and eventually react much more easily than it would otherwise be possible. Both cases require an understanding at the molecular level in order to fully comprehend them. Given the multitude of physico-chemical processes at play, it is absolutely essential to deploy theoretical models to help explain experimental observations. To this aim our team develops methods, algorithms and simulation codes, and applies these (and third-party tools) to build nanoscopic models. Recent and ongoing applications involve the simulation, including temperature effects (by averaging results over many configurations), of: (a) HO_2 reactive uptake on organic aerosols, though the combination of classical molecular dynamics (CMD) simulations and non-relativistic ab initio QM/MM calculations; (b) the XPS spectra of iodide in water droplets, and how valence ionization spectra of chloride and iodide in water droplets varies with water droplets size, though a combination of the full stack of methods developed in the group (polarizable force fields for CMD simulations, and relativistic EOM-IP-CCSD-in-DFT QM/QM embedding); (c) the XPS spectra of HCl and chloride at air/ice interfaces, combining CMD snapshots and relativistic EOM-IP-CCSD-in-DFT embedding; and (d) the solvation of the iodate (IO_3-) ion, employing Car-Parrinello MD (CPMD) simulations due to the lack of appropriate polarizable force fields to describe the solvated ion. The sheer volume of simulations in these examples made the national supercomputing facilities indispensable for achieving our aims.

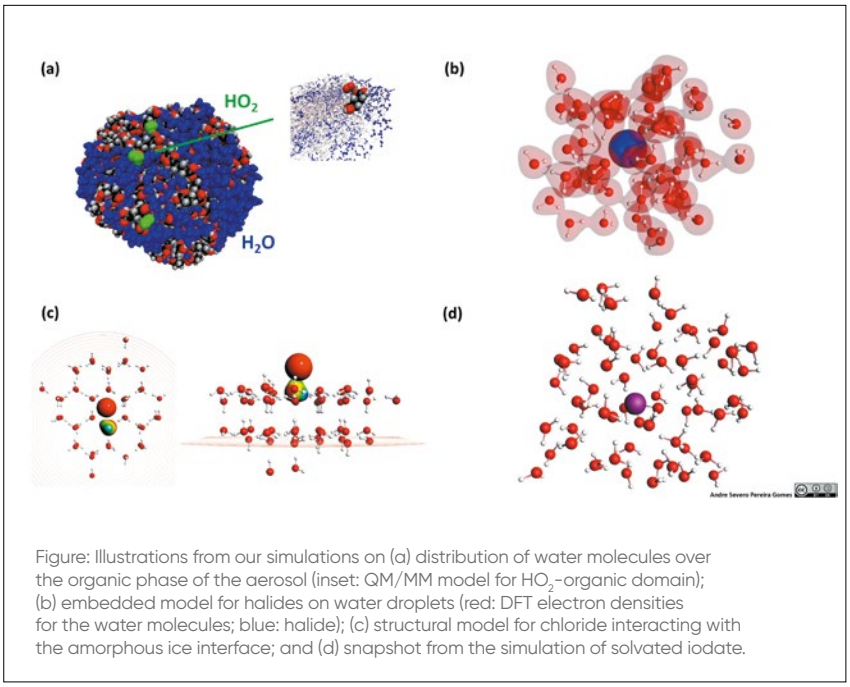


Figure: Illustrations from our simulations on (a) distribution of water molecules over the organic phase of the aerosol (inset: QM/MM model for HO_2-organic domain); (b) embedded model for halides on water droplets (red: DFT electron densities for the water molecules; blue: halide); (c) structural model for chloride interacting with the amorphous ice interface; and (d) snapshot from the simulation of solvated iodate.

CT7 MOLECULAR MODELLING APPLIED TO BIOLOGY **OCCIGEN: 2 MILLION HOURS**



XIAOLING WU,
POST-DOCTORAL FELLOW, UNIVERSITY COLLEGE LONDON, UK
FABIEN CAILLEZ,
ASSISTANT PROFESSOR, UNIVERSITÉ PARIS-SACLAY
AURÉLIEN DE LA LANDE,
CNRS RESEARCH DIRECTOR, UNIVERSITÉ PARIS-SACLAY

Université Paris-Saclay

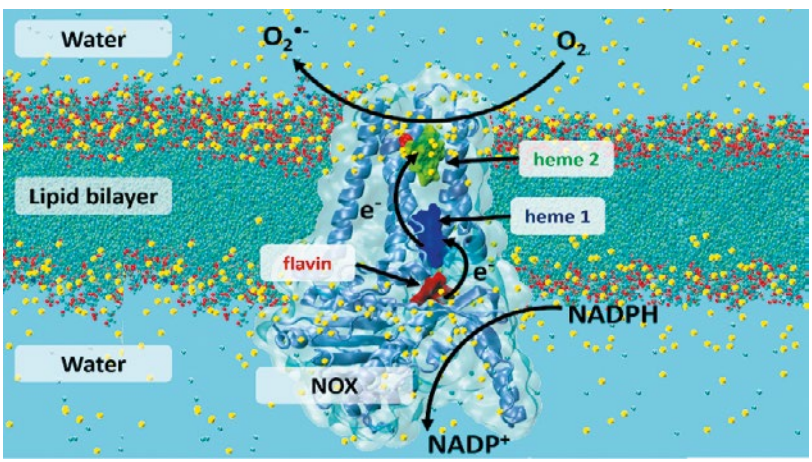
BIOLOGY, CHEMISTRY AND MATERIALS

Numerical simulations reveal some secrets of the molecular bases of immune defense

Cells are experts in shuttling electrons at the microscopic scale to fulfill their metabolic needs. A fascinating example if that of class 2 NADPH oxidases (NOX2) that play pivotal role in immune defense system. NOXs are molecular machineries dedicated to the production of free oxygen species such as the superoxide anion ($O2^{\bullet-}$) that are targeted to destroy pathogens locked in phagosomes. The latter are kinds of lipid-made baskets encaging pathogens. Few in actually known regarding the molecular mechanisms that afford superoxide production catalysis by NOX, even though the first tridimensional structures released since 2017 have started to shade light on this. The electrons necessary to reduce dioxygen are thought to be passed from the exterior to the interior of the phagosome membrane via successive electron hops involving a flavin and two heme cofactors.

The teams from the Institut de Chimie Physique (ICP, Université Paris-Saclay, CNRS) and from the Laboratoire de Biochimie Théorique (LBT, CNRS) have joint forces to unravel some of the secrets of the transmembrane electron transfer, focusing, in a first round, on the inter-heme step. A first challenge was to build a realistic model of a NOX inserted in a lipid bilayer. The model built at LBT comprises 180,000 atoms and appears to be sable over hundreds of nanoseconds of molecular dynamics simulations. In a second step, the ICP teams deployed dedicated computational tools to evaluate for the first time the electron transfer reaction free energy. The team further identified the fluctuating pathways between affording electron tunneling between the two hemes. These results have raised many new fascinating questions to be now addressed.

Our project has benefited from the support of GENCI supercomputers and fomr the DYNAMO Labex. The results have been published in a special issue of Frontiers in Chemistry dedicated to redox enzymes (X. Wu, J. Hénin, L. Baciou, M. Baaden, F. Cailliez, A. de la Lande, 2021, 9, 650651).



NOX are membrane proteins dedicated to the production of reactive oxygen species, here superoxide anions ($O2^{\bullet-}$).

Electrons are shuttled from the NADPH molecule to molecular oxygen via a succession of hops involving the flavin, the heme1 and heme2 cofactors.

MICHEL MASELLA
CEA, BASIC SCIENCE DIVISION,
INSTITUT JOLIOT
LUIGI GENOVESE
CEA, BASIC SCIENCE DIVISION,
INSTITUT IRIG

OTHER APPLICATIONS (COMPUTING, HEALTH, ETC.)

Modeling antobody/antigen assemblies

Awarded by a SANOFI iTech Award 2020

Monoclonal antibodies are promising therapeutic agents against autoimmune diseases, cancers and the COVID-19 disease. In France that field represents an important economical activity, from company start ups to the pharmaceutical group SANOFI, who restructured its R&D center of Vitry Sur Seine to be a major production plant of monoclonal antibodies.

Targeting specific monoclonal antibodies can be routinely achieved, however increasing the antibody affinity as much as desired is a challenging task. The available theoretical tools devoted to it focus on investigating close contact antibody/antigen, AA, local regions. Moreover because of their size, only standard molecular modeling approaches or empirical cost functions are used to quantify the strength of AA interactions. However these approaches rely on crude approximations preventing to reach a high enough level of accuracy.

Our project consists in adding two new steps to standard computational protocols devoted to investigate AA assemblies to further assess their solutions. These steps consist (1) in investigating the AA potential energy surface from Replica Exchange simulations using a polarizable multi-scale molecular modeling approach as implemented in the code POLARIS(MD); (2) in refining the simulation results by means of an efficient quantum chemistry code, BIGDFT, that allows one to investigate full AA assemblies (that comprise at least about 6 000 and usually more than 10,000 atoms). Our project has been awarded by a SANOFI iTech Awards in 2020 and it is granted access to the TGCC supercomputing system IRENE by GENCI in 2020 and 2021 (15 M computational hours each year).

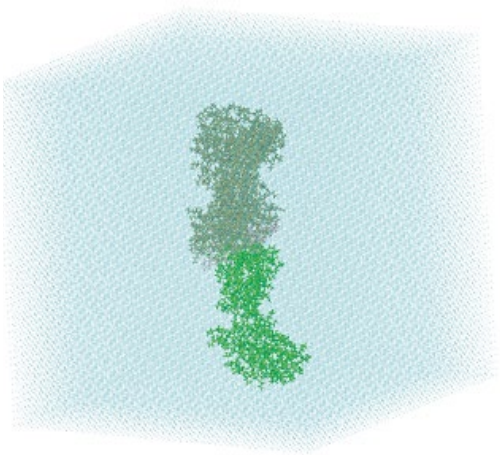


Fig. 1: an AA assembly investigated in aqueous phase using our multi-scale Molecular Modeling, MM, approach (http://biodev.cea.fr/polaris/).

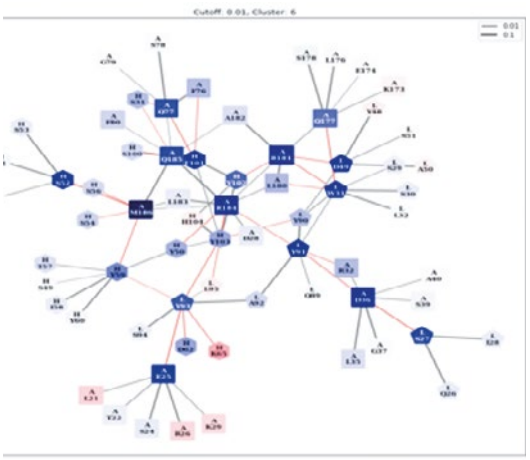


Fig. 2: a graph representation of the interactions within an AA assembly from post processing the MM simulations using the code BigDFT (see http://bigdft.org/). @CEA

CT6 COMPUTING, ALGORITHMS AND MATHEMATICS **JOLIOT-CURIE ROME: 5 MILLION HOURS**

PIERRE JOLIVET,
RESEARCHER,
INSTITUT DE RECHERCHE EN INFORMATIQUE DE TOULOUSE,
CNRS

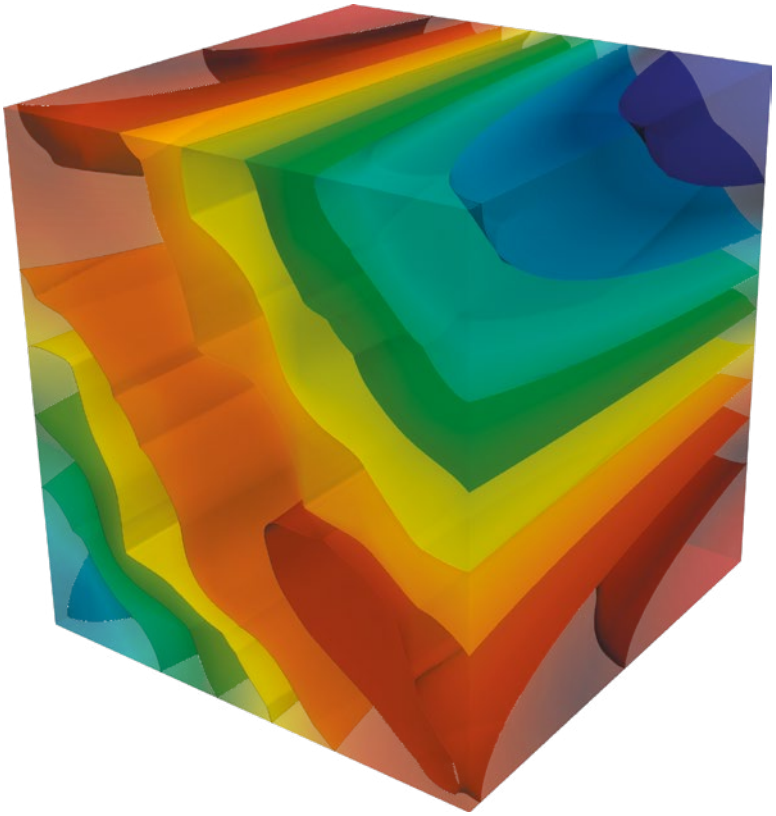
OTHER APPLICATIONS (COMPUTING, HEALTH, ETC.)

Adaptive domain decomposition methods

Domain decomposition methods are based on the divide-and-conquer paradigm to solve linear systems resulting from the discretization of partial differential equations. These methods are from the same class of algorithms as multigrid methods. They are quasi-optimal in the sense that the number of operations required to reach convergence is O(N), where N is the size of the sparse system to solve.

Compared to the slightly superlinear costs of LU or LLT factorizations, one can understand the attractiveness of these hybrid methods. Although the theory of domain decomposition methods is widely studied, there are few implementations available to the scientific community. Our project is centered around such an implementation *(https://github.com/hpddm)*, itself interfaced with numerical libraries such as PETSc *(https://petsc.org)*.

The efficiency of multilevel methods relies on the development of "coarse" grids that let these preconditioners scale, independently of the number of computational units and the complexity of the physical model. These grids can be constructed algebraically, requiring only the linear system to be solved. In cases where this is not possible, information is transmitted by the discretization kernel during the construction of the preconditioner, e.g., finite element elementary matrix, so that the coarse grid adapts to the physics. The theoretical framework of algebraic and non-algebraic methods does not allow to date to certify the convergence of domain decomposition methods for an arbitrary problem. Initially applicable with guarantees only for some specific problems such as symmetric positive definite matrices, recent advances allow us to deal with new problems, such as least squares, adaptively.



Isovalues of the solution of a nonlinear problem (Bratu equation) obtained with PETSc using an adaptive domain decomposition method.

CT10 NEW APPLICATIONS AND MULTIDISCIPLINARY APPLICATIONS OF HPC **JEAN ZAY: 5 MILLION HOURS**

THOMAS WOLF,
SCIENTIFIC DIRECTOR - CO-FOUNDER,
HUGGING FACE

OTHER APPLICATIONS (COMPUTING, HEALTH, ETC.)

BigScience

The acceleration in Artificial Intelligence (AI) and Natural Language Processing (NLP) will have a fundamental impact on society, as these technologies are at the core of the tools we use on a daily basis. A considerable part of this effort currently stems in NLP from training increasingly larger language models on increasingly larger quantities of texts. Unfortunately, the resources necessary to create the best-performing models are found mainly in the hands of big technology giants. The stranglehold on this transformative technology poses some problems, from a research advancement, environmental, ethical and societal perspective.

Inspired by large open research collaborations like the LHC, the BigScience project was started in early 2021 with the aim of demonstrating another way of creating, studying, and sharing large language models and large research artefacts in general within the AI/NLP research communities.

BigScience was created as a one-year long research workshop on large multilingual datasets and large multilingual language models. Today, it brings together more than 900 researchers from 60 different countries and 250 academic and industry labs. Thirty different working groups are dedicated to the areas of data, modeling, engineering and scaling, evaluation as well as assessing ethical and legal implications and social and environmental impact related to large language models, making it among the largest collaborative open science projects in AI to date.

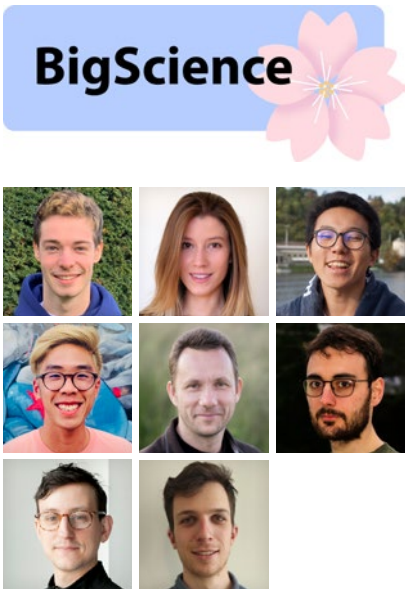
As detailed below, the workshop is currently creating several research artifacts that will be shared with the research community:

- A multilingual dataset
- A large multilingual Language Model (100-200B parameters) trained on the powerful French supercomputer Jean Zay (5M GPU hours granted for BigScience)
- Software tools, e.g. dataset filtering, model off-loading, etc.
- Documentation of the processes, results, protocols, datasets, and tools developed in the course of the project

The main large language modeling experiments as well as complementary efforts are being conducted on the Jean Zay supercomputer infrastructure (5 million GPU hours in total that were granted to the BigScience project).

READ MORE ABOUT BIGSCIENCE

- BigScience website
- Intro, short history, founding members, organization
- Find research artifacts, collaborations and events organized in 2021
- Read more about the BigScience working groups



From left to right and top to bottom:
Hugo Laurençon (Machine Learning Engineer, Hugging Face),
Lucile Saulnier (Machine Learning Engineer, Hugging Face),
Thomas Wang (Machine Learning Engineer, Hugging Face),
Victor Sanh (Research Scientist - Lead, Hugging Face),
Stas Bekman (BigScience team Engineer, Hugging Face),
Pierre Colombo (Post-doctoral fellow, L2S - Centrale Supelec),
Sylvain Viguier (Director of Applications, Graphcore),
Roman Castagné (PhD Student, ALMAnaCH - INRIA Paris)

GENCI AND ITS ENVIRONMENT

CLUSSTER: CLOUD, EDUCATION AND INDUSTRY

The CLUSSTER project, Sovereign Unified Cloud of Services, Technologies and Infrastructures, aims to develop and strengthen the French and European Cloud domain by being part of the CLOUD acceleration strategy of the Directorate General for Enterprise (PIA4). CLUSSTER brings together 10 French partners, including major French academic (GENCI, IDRIS/CNRS, INRIA, CEA-LSCE) and industrial (Atos, Activeeon, OVHcloud, CS GROUP, Qarnot, Hubblo) players to create a unique and scalable research cloud. The initial purpose, which will focus to meet needs in Artificial Intelligence, will be extended to HPC and quantum fields later. The project will also endeavor to be a gateway to access infrastructure and services available in Europe thanks to its integration with the federation services of the European cloud platforms GAIA-X and EOSC (European Open Science Cloud).

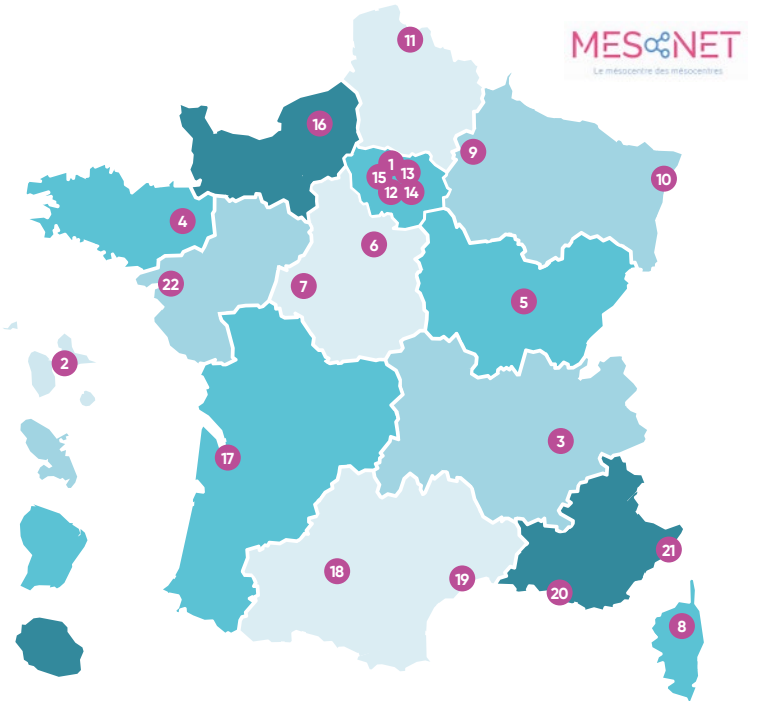
Funded with a budget of €15.8M over 3 years, CLUSSTER is based concretely on the implementation of a unified cloud portal to offer a complete visibility, both of known sovereign academic and industrial infrastructures, as well as added-value services (Support, business expertise, training (including for students and teachers), technology watch) in AI, to ensure a unique continuum between open and confidential research and commercial activities.

MesoNet: THE REGIONAL MESOCENTERS FEDERATION

The MesoNet project, bringing together 21 regional mesocentres and coordinated by GENCI, officially started on October 1st, 2021 for a period of six years and a consolidated budget of M€. This project benefits from a national funding managed by the National Research Agency under the "Investments for the Future" program with the reference "ANR-21-ESRE-0051".

The primary objective of the project is to foreshadow the establishment of a national research infrastructure for mesocentres. MesoNet shall increase the visibility of mesocentres at French and also European level, in connection with the European infrastructure EuroHPC and the French Competence Center. This infrastructure will provide industrial and academic communities as well as students with resources in HPC intensive computing but also in new approaches such as artificial intelligence and quantum computing. The investments made will cover the whole spectrum, from beginners to national and European needs.

The importance of training and of the skills that will be developed there, in diversity and in quantity, must be emphasized. This sector is indeed a source of jobs for the future, and the training of new generations to develop computing skills is an essential issue.



MesoNet PROJECT PARTNERS

1	GENCI	
2	Université des Antilles	
3	CINAURA (Université Grenoble, Alpes, FLMSN)	
4	GIP numérique Bretagne	
5	Université de Bourgogne Franche-Comté	
6	Université d'Orléans Fédération CaSciModOT	
7	Université de Tours Fédération CaSciModOT	
8	Université de Corse Pasquale Paoli	
9	Université de Reims Champagne-Ardenne	
10	Université de Strasbourg	
11	Université de Lille	
12	Université de Paris Saclay	
13	Centrale Supelec	
14	ENS Paris Saclay	
15	Paris sciences et lettres (dont Observatoire de Paris)	
16	CRIANN (Rouen)	
17	Université de Bordeaux	
18	Université de Toulouse (Calmip)	
19	Université de Montpellier (Meso@LR)	
20	Aix-Marseille Université	
21	Université Côte d'Azur	
22	Centrale Nantes	

COMPETENCE CENTER AND SiMSEO FOR SME & STARTUPS

The SiMSEO Project to support SMEs in computational simulation has completed its sixth period (October 1, 2020 to September 30, 2021). SiMSEO allows SMEs and mid-cap companies to get support, including financially, to carry out a proof of concept around digital simulation.

Despite the complex health situation, GENCI and the regional platforms have raised awareness among manufacturers through various initiatives: workshops, conferences, "B2B" business meetings, canvassing of agencies acting as intermediaries (CCI, competitiveness cluster, regional stakeholders). The important point to note is the involvement of SiMSEO in the European Competences Centers project led by Teratec, Cerfacs and GENCI which results in the actions of SiMSEO being nested in the French Competence Center. The European Competence Center project having an operating period of 2 years, this led us to ask the DGE for an authorization for the two-year extension of SiMSEO, i.e. until September 30, 2022.

In total, since the operational launch of SiMSEO's "Local Support for SMEs" program in May 2016, more than 2,200 SMEs have been made aware, 135 SMEs have taken steps to set up a project and 72 projects have been launched.

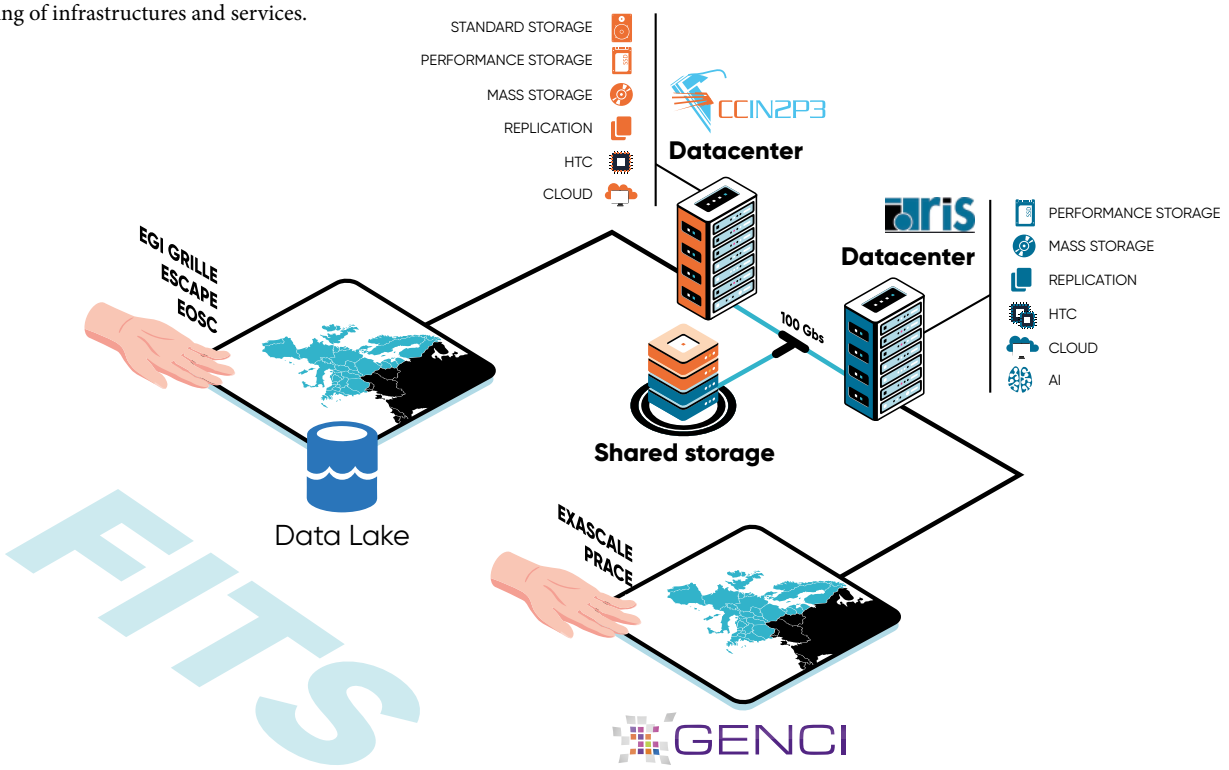
On the *Rendez-vous Carnot* trade show, on November 17 and 18, 2021 and *Big Data & AI Paris* on September 28 and 29, 2021

FITS PROJECT: CNRS FEDERATED DIGITAL SERVICES FOR RESEARCH INFRASTRUCTURES

MESRI research infrastructures will have to deal with an exponential increase in the amount of data they produce. The dichotomy between experimental data and data from digital simulation, each of which requires digital processing and analysis resources with very different technical architectures, has come to an end. Policies on open science and open data, whether national or European, are creating additional needs, while the need to contain digital costs is leading to a policy of rationalization and pooling of infrastructures and services.

The ambition of the CNRS FITS project is to federate, thanks to its two national computing centers (IDRIS and CC-IN2P3), their services and know-how, through the implementation of a distributed infrastructure for storage, processing, and the provision, dissemination, and enhancement of data, hosted in environmental conditions with a low carbon footprint.

This infrastructure, based in part on GENCI's equipment at IDRIS, will provide the infrastructure with computing and data processing resources combining high-performance computing and high-speed computing, supercomputing with graphics gas pedals and data processing farms, containerization and cloud computing. This platform will be an essential component of the European Open Science Cloud (EOSC).



PRACE-6IP

PRACE, the Partnership for Advanced Computing in Europe, has been established as a pan-European ESFRI Research Infrastructure providing state-of-the-art computing services to enable world-class research on world-class high-performance computing systems.

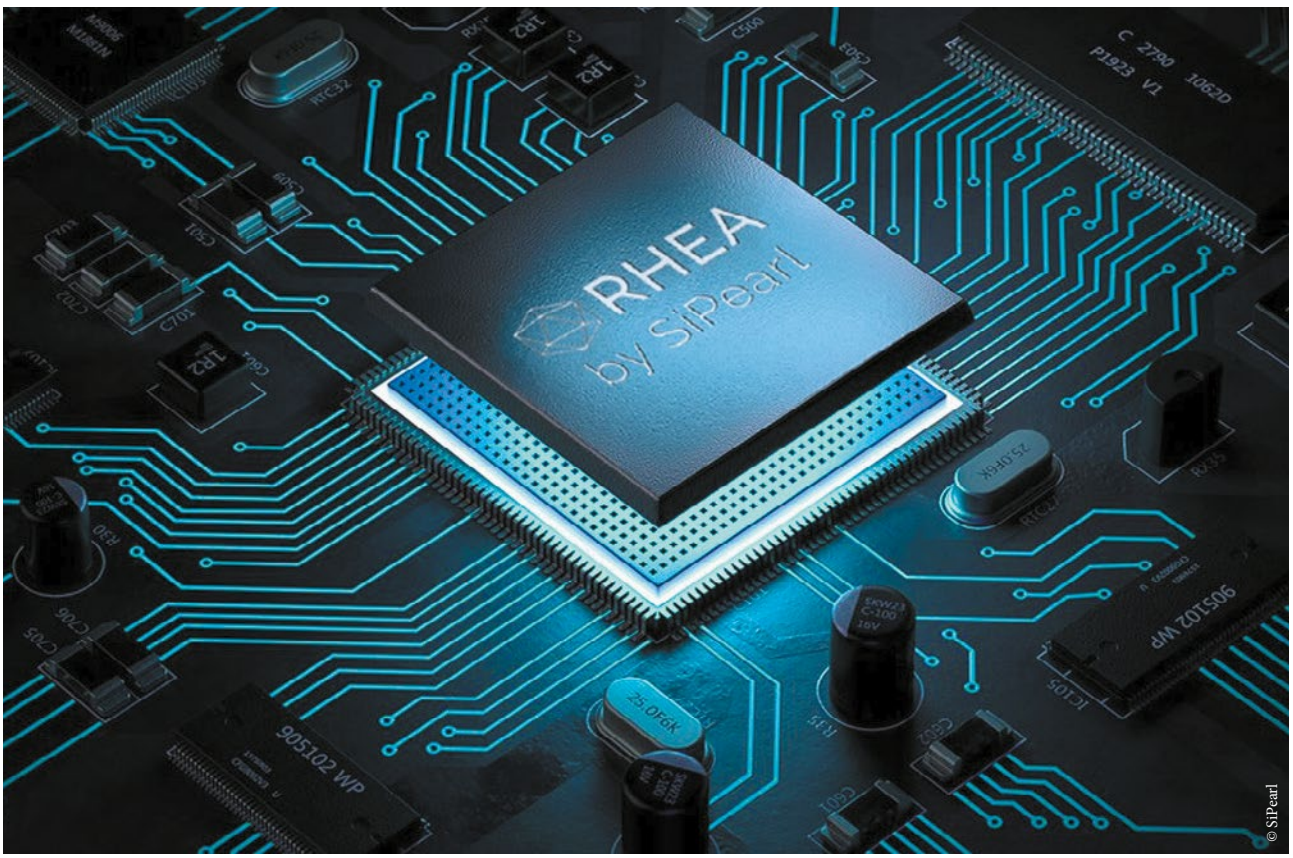
PRACE aisbl, its 26 members along with EUDAT and GÉANT collaborate in the PRACE-6IP project. This 6th Implementation Phase will be the last one funded by the European Commission, in the future it will be replaced by a set of projects dedicated to specific services, funded through the EuroHPC JU. PRACE-6IP project was designed to build on and seamlessly continue the achievements of PRACE and start new innovative and collaborative activities. 2021 was supposed to be the last year, but some activities, such the 2021 and 2022 editions of EuroHPCSummitWeek, will be extended until end of June 2022 before EuroHPC JU took over some activities.

During this year PRACE-6IP project have also collaborated with the ETP4HPC, Centres of Excellence (CoEs) and other European and international organisations on future architectures, training, application support and policies, with other e-Infrastructures or projects such as EUDAT and FENIX (offering their resources in PRACE calls and working on AAI) or GÉANT or large-scale research facilities such as ESRF, SKA and CERN and foster relations to the European Open Science Cloud (EOSC). It also continued independent joint technology watch, advanced training which has so far provided close to 70,000 person-training days for participants coming from 96 countries, and expanding the network of PRACE Training Centres, and Promoting the adoption and use of HPC by industry and new user communities and offering special services to SMEs.

MORE INFO ON PRACE

www.prace-ri.eu

UPDATE ON THE EUPEX/SGA2 FR PROJECT



© SiPearl

The EUPEX project, EUropean Pilot for EXascale, is part of the vision to developp sovereign technologies that can equip future European Exascale architectures. Cofunded by the EuroHPC Joint Undertaking as well as France (via Bpifrance), Germany, Italy, Greece, the Czech Republic and Croatia, its budget is €40.8 million for 4 years for a total of 19 industrial and academic partners (including in France Atos, the CEA, Inria, GENCI and SME Cybele Tech). EUPEX aims to deploy and validate the first European platform for HPC integrating all the European technologies previously funded by Europe, from the processor resulting of the 1st phase of the European research project EPI (European Processor Initiative) SGA1 to the software layer up to the applications. The EUPEX project, which started at the start of 2022, will initially rely onto the innovative A64FX platform installed on Joliot Curie at the TGCC, while waiting for the availability of the Rhea processor from SiPearl company. This platform will allow developers to port their applications onto a processor with characteristics similar to the European Rhea processor.

In the continuity of the EPI SGA1 project, Europe continues to support the definition of the 2nd generation of the European processor as of an accelerator and commits funding €70 million to the EPI SGA2 project which will start in February 2022 for 3 years.

GENCI, A CIVIL COMPANY

WOMEN AND MEN WORKING TO SUPPORT RESEARCH

—— **GENCI continued the efforts initiated in 2020 to dematerialise internal processes and improve them continuously.** GENCI continued to dematerialise financial operations by processing and validating invoices via SAGE automation accounting. This system ensures that invoices are available in dematerialised format and that all actions (validation dates and validator) are recorded for each of the company's expenses. Internal control is thus strengthened and the risks of fraud or omission are considerably reduced.

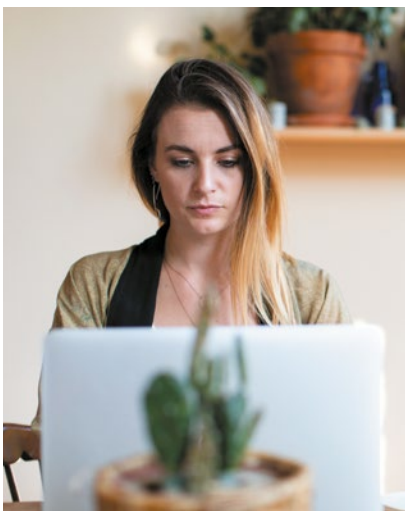
Following an internal review and a multiplication of operations with the computing centres, a matrix was created to list the contractual commitments and provide operational and financial monitoring.The originality of this approach lies is based on the fact that the tool is accessible to all GENCI staff (legal, financial, technical and operational) or the computing centre concerned.

Finally, with the aim of continuously improving processes, GENCI has deployed a new HR module, "Pagga", developed by the company Lucca, which enables employees to receive their payroll sheets in a secure, individualised "safe" by electronic means.

—— **The measures implemented in 2020, relating to the COVID-19 sanitary crisis, have been extended until September 2021.** A safety protocol has been put in place and applies to staff as well as to any external visitors.

GENCI had no difficulty in ensuring continuity of service as teleworking had been implemented by 2019. Based on this organisational success, telework was extended on the initiative of the employer and after extensive consultation with the employees, to two days per week from 1 September 2021.

In addition, at the beginning of 2021, employees were allocated a financial envelope of up to 450 euros per employee to cover the cost of office equipment needed for regular teleworking at home.



—— **In terms of human resources, the year was marked by several events.** Firstly, on 2 June 2021, the Partners unanimously approved the re-election of Philippe Lavocat as CEO for a period of five years.

Following the resignation of the employee representative in mid-August, new elections for the Social and Economic Committee were organised. These were held in October. As no candidates were presented, an omission statement was drawn up.

The workforce has been established at twenty people for 2021. GENCI recruited two new employees on permanent contracts for the positions of Head of Communications (April) and Administrative Project Manager (April), as well as an interim recruitment for the position of Exascale Project Manager (February). At the same time, the Competence Centre/MesoNet project manager left in mid-August.

—— **In the area of public procurement,** the result of the competitive dialogue procedure for the renewal of CINES' computing resources was disputed in court by one of the unsuccessful candidates. GENCI's teams, supported by those of CINES, carried out a very important analysis in order to contest the arguments raised by this candidate in the context of a pre-contractual referral. The court hearing was held on 19 July 2021. The judge's order of 25 July dismissed all of the plaintiff's claims.

—— **In addition, GENCI finalized the implementation of the processes resulting from the RGPD review** of the subcontracting relationship between GENCI and IDRIS and the users of the supercomputers/responsible for the processing of personal data. The review carried out by GENCI having identified the 1st and 2nd level subcontractors (respectively GENCI and the centres), the documents for the compliance of the user/IDRIS/GENCI relationship for the allocation of computing resources have been validated by the parties concerned.

This work carried out with the CNRS and IDRIS teams to address an urgent requirement will now be continued with the two other computing centres (TGCC and CINES) in 2022.

INTERNAL ORGANIZATION IN 2021

MANAGEMENT COMMITTEE

Philippe LAVOCAT
CEO

Edouard BRUNEL
General Secretary

Jean-Philippe PROUX
Operations and Security Officer

Stéphane REQUENA
CTO and Innovation Manager

Marie-Hélène VOUETTE
Partnership Manager
Institutional Relationships Advisor

ADMINISTRATIVE AND FINANCE DEPARTMENT

Maïté CAMPEAS
Executive Assistant

Imène LITIM
Administrative Assistant

Laetitia PHO
Administration and Finance Manager

Marieke PODEVIN
Senior Legal Officer
Data Protection Officer

Rasa VAICIEKAUSKAITE FALLAHZADEH
Administrative project manager

COMMUNICATION

Nicolas BELOT
Communication manager
and European relations

Annabel TRUONG
Communication Officer

TECHNICAL AND OPERATIONS DEPT.

Christelle PIECHURSKI
HPC Project Officer with responsibility
for the Technology Watch Unit

Elise QUENTEL
National and European Projects Manager:
Equip@meso, SiMSEO

Philippe SEGERS
European Projects Manager

Corinne BEAL
Exascale Project Manager

Delphine THEODOROU
Project Operations Manager

Pascal VOURY
Project Operations Manager

Abraham LUNDA
Technical- Commercial Projects Manager:
Competence Centre

COMMITTEES MEMBERS AND OFFICIAL BODIES

AT 31/12/2021

CEA: Commissariat à l'Énergie Atomique et aux Énergies Alternatives. **CNRS:** Centre National de la Recherche Scientifique. **France Universités.** **Inria:** Institut national de recherche en informatique et en automatique. **MESRI:** Ministère de l'Enseignement Supérieur, de la Recherche et de l'Innovation.

Membership of the GENCI Council

State and MESRI representative: Mr Laurent Crouzet - Mr Nicolas Dromel. CEA representative: Mrs Maria Faury - Mr Hervé Desvaux. CNRS representative: Mr Ali Charara - Mr Denis Veynante. Universities' representative: Mr Guillaume Gellé - Mr Olivier Simonin. Inria representative: Mr Jean-Frédéric Gerbeau.

Membership of the Administrative and Financial Committee (CCAF)

State and MESRI representative: Mr Antoine Perrang, *Chairman of CCAF.* **CNRS representative: Mrs Anne-Françoise Duval. CEA representative: Mr Rémi Keller. Inria representative: Mr Vincent Heyer. Universities' representative: Mr Michel Dellacasagrande.**

Membership of the Contracts Audit Committee (CM)

State representative: Mr Philippe Ajuelos, *Deputy - Head of the digital development department - National Education Ministry, Chair of the Contracts Audit Committee* - **Mrs Lara Montantin,** *senior lawyer - Direction générale de la recherche et de l'innovation du Ministère de l'Éducation Nationale.* **Universities' representative: Mr Hervé Celestin,** *Head of Administration and Finances Service.* **CEA representative: Mr Eric Stehle,** *Head of Commercial Service-Cea-Saclay* - **Mr Thibault Pelletier,** *Head of Referential Service and Head of Contracts Audit Committee - at CEA.* **CNRS representative: Mr Sébastien Turci,** *Managing Director for purchases & innovation* - **Mrs Marie-Laure Colin,** *Head of the Juridical Rules Department - Directorate for Legal Affairs.*

Technical Advisory Committee (CT)

State and MESRI representative: Mr Laurent Crouzet, *Head of the Digital Services and Infrastructures Department.* **CEA representative: Mrs France Boillod-Cerneux,** *Division for Fundamental Research* - **Mr Emeric Brun,** *Directorate for Nuclear Energy* - **Mrs Christine Menaché,** *Head of TGCC.* **CNRS representative: Mr Michel Daydé,** *Scientific Delegate* - **Mr Pierre-François Lavallée,** *Director of IDRIS.* **Universities' representative: Mr Francois Bodin,** *Professor @ University Rennes1* - **Mr Boris Dintrans,** *Director of CINES.* **Inria representative: Mr Jean Roman,** *Deputy Scientific Director - Research Directorate for Applied Mathematics, Computing & Simulation* - **Mr Lucas Nussbaum,** *Responsable du programme plateformes d'expérimentation à la Direction Générale Déléguée à l'Innovation.*

Committee for Strategic Orientations on Investments (COSI)

Committee with responsibility for advising and providing assistance to GENCI in its investment strategy covering in particular the compilation of a multi-year investment plan based on the indications given by the MESRI scientific committee and guiding the work of the CT and CCAF.

State and MESRI representative: Mr Laurent Crouzet, *Head of the Numerical Services and Infrastructures Department.* **CEA representative: Mr François Robin,** *CEA DAM-IDF Directorate* - **Mr Christophe Calvin,** *CEA Fundamental Research Directorate.* **CNRS representative: Mr Ali Charara,** *Director of CNRS-Digital Sciences & their Interactions Institute* - **Mr Denis Veynante,** *Chairman of the Steering Committee of the Compute & Data Mission.* **Universities' representative: Mr Olivier Simonin,** *Chairman of National Polytechnique Institute.* **Inria representative: Mr Jean Roman,** *Deputy Scientific Director - Research Directorate for Applied Mathematics, Computing & Simulation.*

A huge thank-you goes to the authors and contributors for your time and the energy you have dedicated to this Annual Report outlining all the work of GENCI during 2021.

It is only thanks to the people in this report, as well as many others, that GENCI is able to achieve its objectives and be part of the emergence of new possibilities every year.

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