



HPC at the service of knowledge

**ANNUAL
REPORT**

20





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3

Computing Centers, for a total of 53.5 PFlop/s

CINES
OCCIGEN supercomputer
3.5 PFLOP/S

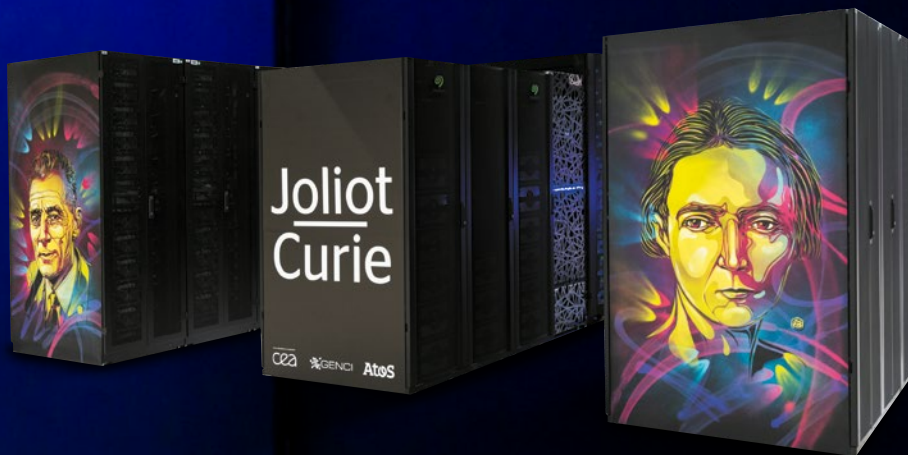
IDRIS
JEAN ZAY supercomputer
28 PFLOP/S

TGCC
JOLIOT-CURIE supercomputer
22 PFLOP/S

5

Shareholders

MESRI | CEA | CNRS | CPU | Inria



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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**“Supercomputers considered
by our partners and competitors
as essential for the advance of research
and knowledge, and for the emergence
of innovative ideas.”**



2020 or how, even in lockdown, GENCI continued preparing the future

EDITORIAL BY PHILIPPE LAVOCAT, CEO OF GENCI

2020 is coming to an end. Thank goodness, some would say, scarred by the ongoing health crisis. Whilst lockdown might mean “non-movement” from a Taoist viewpoint, it has not been synonymous with inaction for GENCI and its Associates, in fact quite the contrary! It is very much in the nature of human beings to do everything possible to keep hope alive and look to the future to come back stronger. GENCI is no exception to the rule! With the commitment of its team and working closely with the teams at the three national computing centers, GENCI has adapted to remote working to ensure continuity of service and achieve its strategic objectives.

You will find most of GENCI’s actions at regional, national and European level in this annual report. I would however like to focus my remarks on the importance of preserving and developing major research infrastructures, tools and national assets that are of strategic importance for scientific and economic competitiveness. GENCI was among the few facilities able to continue their operations. GENCI was also above all able to respond in a matter of days to national, European and global requests for

“Urgent Computing” in the fight against COVID19 by supporting 40 research projects. These projects were given priority and rapid access to its high-performance computing and massive data processing resources.

At a time when France is preparing, in collaboration with the European Commission and 33 European States, to purchase a supercomputer capable of carrying out almost a billion-billion of operations per second, it is worth remembering that such tools are considered by our partners and competitors as vital to the development of research and knowledge, and to the emergence of innovative ideas.

There is still a lot to be said about the continuity of the actions carried out in 2020 by the staff at GENCI and the computing centers, whom I would like to thank wholeheartedly. You will read about them in the pages of this report. My last word will be to the Associates who, in the current national mindset of doubt, have encouraged GENCI to take the risk of projecting into the future, the true source of future success and advances in knowledge!

2020 as seen by GENCI's Shareholders



Jean-Frédéric Gerbeau
DEPUTY CEO FOR SCIENCE AT INRIA



CONSTANT GROWTH IN CAPACITY

2020 saw Inria's project teams make further progress in the use of deep learning methods on GPUs, in the context of the Jean-Zay challenges. This included work on the creation of realistic human videos by disjointed coupling of appearance and movement, as well as work on high-resolution modelling of the distribution of plant species to understand the fundamental mechanisms governing ecosystems.

Similarly, as part of the Joliot-Curie challenges, work in electrophysiological modelling of the heart, with a resolution almost at the scale of the cell, was carried out using 200,000 computing cores with a mesh of 11 billion elements. This work, which is part of a EuroHPC project, will produce code that can be deployed on future exascale computers.

Finally, Inria has been involved in the Exascale France Project led by GENCI for the code design and application optimization aspects. ■



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

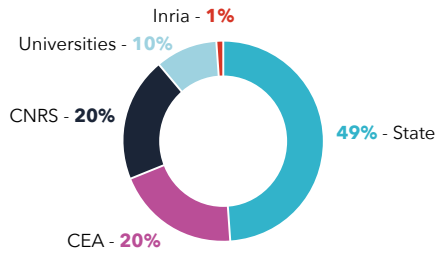


SUCCESSES DESPITE THE CRISIS

It is difficult to talk of 2020 without referring to the COVID-19 crisis. In this context, GENCI and the computing centers demonstrated truly remarkable reactivity in continuing to provide quality service for researchers. The Joliot Curie computer, operated by TGCC, very quickly granted priority access to part of its computing resources for European research teams engaged in the fight against COVID-19.

In scientific terms, there were also successes and a team from CEA (DRF/Joliot and DRF/IRFU) won 2nd place among the 19 international teams entered in the "Brain FastMRI Challenge" organised by Facebook Artificial Intelligence Research and NYU Langone Health, with the objective of comparing performances of various neurone network architectures using subsampled MRI data, corresponding with faster examinations such as could be achieved in the future.

These cutting edge results were obtained very quickly (within 15 days) thanks to the use of the Jean Zay computer and the dynamic access reserved for the French Artificial Intelligence community. ■



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



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



RAPIDLY MOBILISABLE RESOURCES

The deployment of the Jean Zay computer is not just about the entry into service of the first converged high-performance computing / artificial intelligence (AI) architecture in Europe. It is also the moment of the successful arrival within the national centers and the world of high-performance computing (HPC) of the artificial intelligence community and its applications. With the increased flexibility of the dynamic access modes, this success has exceeded expectations and to date there are more requests to open accounts for AI than for HPC.

At the same time, the CNRS has welcomed the success of the FITS project under the Equipex+ call for future research investments. Based on its two national computing centers, CC-IN2P3 and IDRIS, with the participation of GENCI, it aims to meet the computation, storage and data processing needs of the Very Large Research Infrastructures (TGR), such as the SOLEIL synchrotron, presaging new uses of national IT resources. ■

NEW USES FOR THE NATIONAL COMPUTING RESOURCES

2020 was a year marked by the health crisis and the fight against COVID-19 in which our higher education and research establishments were fully engaged. This was a perfect illustration of the need to have powerful computing resources that can be quickly mobilised, to have teams of computer support engineers working closely with researchers in the use of these, as well as for guiding students and young researchers towards HPC by means of dedicated training to prepare the future.

As part of this mobilisation, the OCCIGEN supercomputer hosted by CINES, was made available for urgent COVID-19 simulations, with 5 priority projects using 17 million hours. The computing support team worked alongside the researchers and these urgent computing mode simulations once again highlighted the importance of HPC in crisis situations, such as was also the case in 2009 with the computing of the aftershocks of the Aquila earthquake in Italy, using the earlier JADE supercomputer at CINES.

Numeric simulation has thus become a vital tool for research and decision making and GENCI and its partners, including CPU and through it all the universities, higher education and research establishments it represents, are firmly committed to innovative research and are at the heart of today's societal challenges. ■

What they say about us



January 2020: Jean Zay captures the imagination of the general and specialist press:

French AI researchers finally have their own supercomputer

Jean Zay, the new computer inaugurated Friday 24 January in Saclay, doubles our country's total computing power. It is the first supercomputer specially designed for the needs of artificial intelligence research.

[Les échos.fr rubrique Idées](#)

"With the Jean Zay supercomputer, France and Europe now have their first "converged" computer, capable of handling conventional HPC and the specific needs of artificial intelligence."

[Les échos.fr rubrique Idées](#)

Supercomputer inaugurated in Essonne: "This is a revolution", for Philippe Lavocat, CEO of GENCI.

[France Inter](#)

Petaflops taking on COVID-19.

[rfi.fr](#)

At the beginning of March, support for projects in the fight against COVID-19 was put in place and relayed in the media, on the website of the Ministry of the Armed Forces, on the French Tech thematic network:

This call for projects from the Ministry of the Armed Force, launched by the Defence Innovation Agency (AID), as part of the Government anti-COVID-19 plan, is for receiving proposals in the fight against the COVID-19 pandemic. It is focussed on research into innovative solutions.

[Defense.gouv.fr](#)

COVID-19: Finding innovative solutions to unblock the healthcare system is the objective of the Coalition Innovation Santé.

[Reseau-healthtech.fr](#)

Calls for Europe and France projects in the fights against COVID-19

IRCE Research and Communication
Institute on Europe

[irce-oiing.eu](#)

Researchers from the high performance computing world take up the fight against COVID-19 with the Jean Zay supercomputer, with the research project of Jean-Philip Piquemal in the forefront.

[biotechinfo.fr](#)

In fighting effectively against the COVID-19 virus, we need to recognise it, understand it, know how it is constructed and thus discover its weaknesses.

This is the task being taken up by very many researchers around the world, and in particular at Sorbonne University in collaboration with the Institut Pasteur. Several researchers (Sorbonne Université, Conservatoire National des Arts et Métiers, Université de Limoges, University of Texas in Austin, University of North-Texas and Washington University in Saint Louis) involved in this project are going to get priority - urgent computing - access to the Jean Zay supercomputer, one of the most powerful in Europe and built by Hewlett Packard Enterprise.

[informatiquenews.fr](#)

COVID-19. High Performance Computing researchers take the fight to the virus thanks to the Jean Zay supercomputer

[sorbonne-universite.fr](#)

Supported by Sorbonne Université, the COVID-HP project was selected on 3 April to gain access to the supercomputing resources of the Prace European consortium. For six months it will be simulating the interactions between the SARS-CoV-2 virus and potential medical drugs at the atomic scale. A high resolution is possible thanks to the Tinker-HP software which integrates models inspired by quantum physics.

[industrie-techno.com](#)

June-July, the start of production period is announced for the Jean Zay extension:

Grands Challenges applications for the Jean Zay extension

The start of production period for a new supercomputer or its extension, in this case the HPE Jean Zay supercomputer which has had its GPU capacities more than doubled, provides an opportunity for the so-called "pilot" academic and industrial users, to be able to access computing resources that could include the computer's entire capacity or that of a partition, enabling the performance of very large scale simulations, the so-called "Grands Challenges".

[recherche.cnam.fr](#)

What our partners say about us:

International research is getting organised against COVID-19 and it needs weapons up to the task. The massive computing power of the Jean Zay supercomputer is thus being made available to various molecular modelling or diagnostic tool projects.

[cnrs.fr](#)

Two of the most powerful supercomputers in France, Joliot-Curie, operated by TGCC (Très Grand Centre de Calcul) at CEA and Occigen at CINES (CPU National Computing Centre), have for several weeks been allocating priority access to a large part of their computing resources to European research teams involved in the fights against COVID-19.

[cea.fr](#)

A super-powerful supercomputer on the Paris-Saclay Campus

[universite-paris-saclay.fr](#)

Computing centers speak out in the fight against COVID-19:

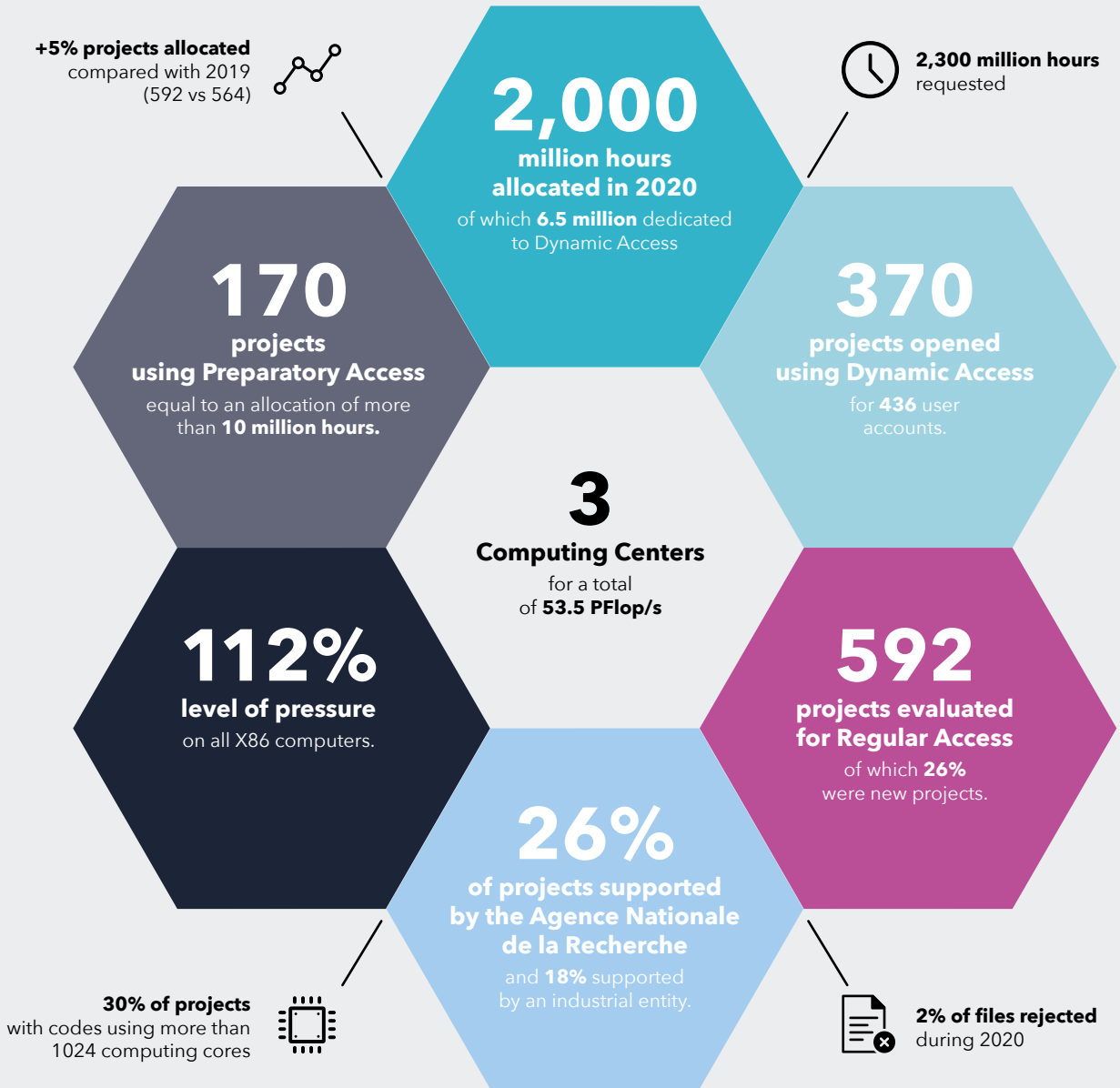
GENCI, CEA, CPU and Atos are arming European scientist with High Performance Computing for their fight against COVID-19.

[cines.fr](#)

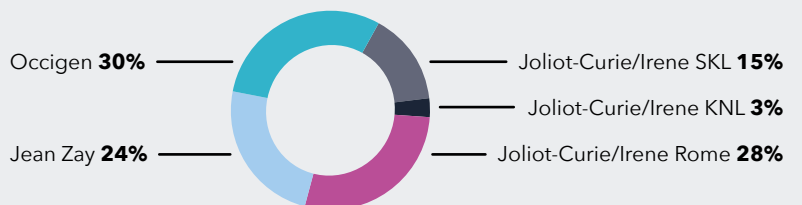
IDRIS is actively involved in research into COVID-19: Press review

[idris.fr](#)

2020 IN FIGURES



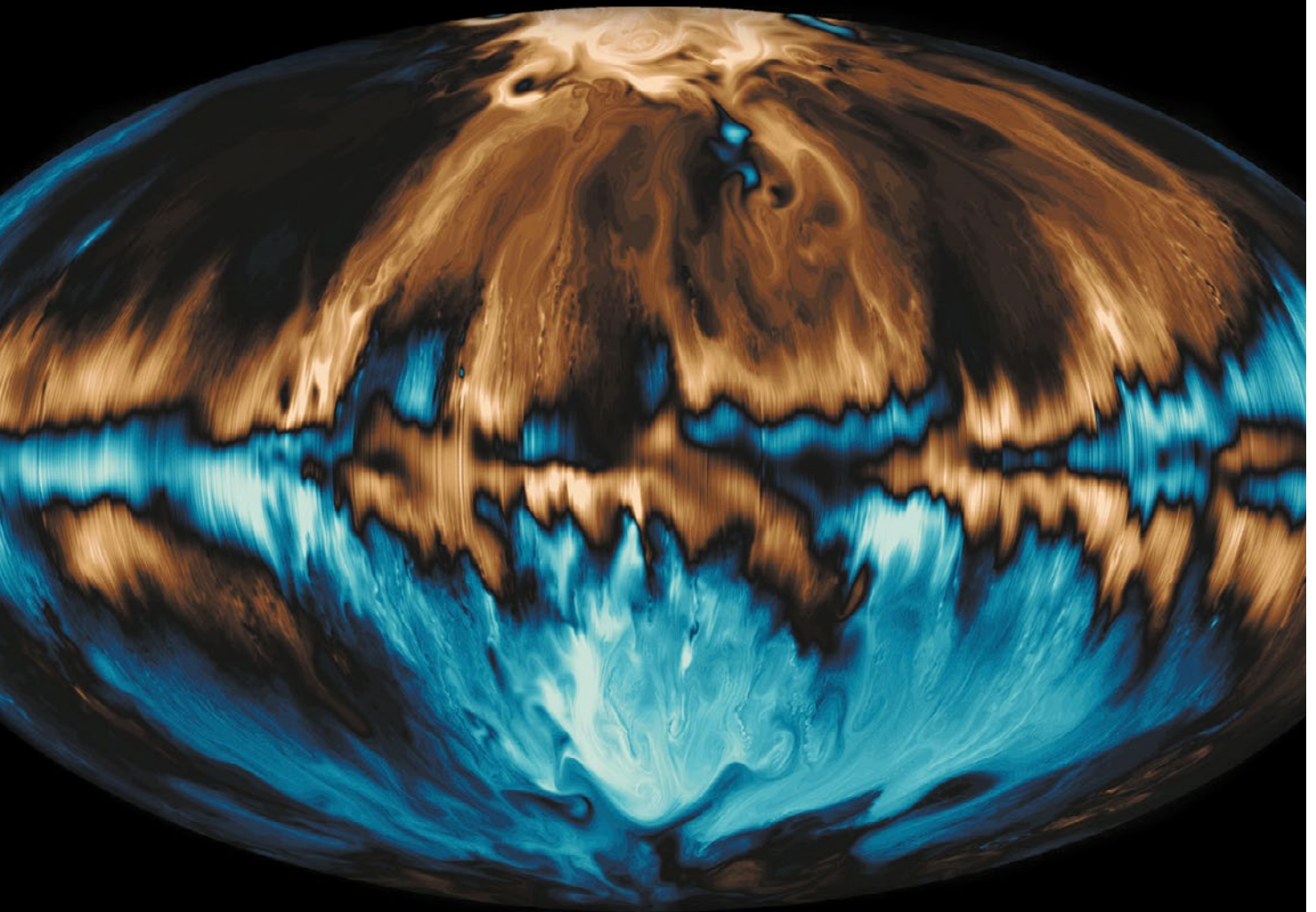
Allocation of hours allocated in 2020
per computer/partition (X86 technology)



**SURFACE OF THE EARTH CORE,
IN THE RADIAL MAGNETIC FIELD.**

This Aitoff cartographic projection, produced on **TURING** and **OCCIGEN**, shows the whole of the globe's surface. The gold and blue colours respectively indicate magnetic fields orientated either towards the exterior or towards the interior of the core.

This numerical simulation of the radial magnetic field of the earth's core was carried out by the Institut des Sciences de la Terre and the Observatoire des Sciences de l'Univers in Grenoble.



2020 highlights

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A year of action at all levels!

BY PHILIPPE LAVOCAT, CEO OF GENCI

AT THE EUROPEAN LEVEL

GENCI has worked for PRACE and EuroHPC cooperation and has been involved in preparations for the French bid to host and operate an Exascale machine: the French organization is now in place. GENCI is working as a partner of the French HPC Competence Centre co-piloted by Teratec and Cerfacs, in charge of transferring know-how to the industrial sector.

GENCI has joined as a member of the EOSC-Europe initiative: combining the scientific orientations of PRACE with the societal and economic aims of EuroHPC by realizing the Open Science vision of EOSC! GENCI contributed to the definition of the EUPEX project proposal: to develop prototypes of sovereign computing resources. On this theme, GENCI worked to achieve the success of first phase of the EPI project aimed at creating a European processor and participated in the European response to the EuroHPC call for projects for the development of a hybrid HPC/quantum platform (HPC-QS).

AT THE NATIONAL LEVEL

GENCI has worked with the CNRS on the definition of the PIA3 FITS project, developed to prepare the processing of data from large research instruments (e.g. SKA telescope array, TGIR (synchrotrons)). GENCI has acquired storage resources for the CINES and IDRIS, completed the Joliot-Curie partitions at the TGCC and started competitive consultations for the renewal of

the CINES machine. Total capacity now exceeds 50 PF. More than 2 billion computing hours were allocated to 1,000 research projects, including 400 in AI. The scientific results of the "Grand Challenges" on Jean Zay testify to the quality of the work carried out jointly with the centers to offer a range of powerful computing resources.

AT THE REGIONAL LEVEL

Cooperation with the mesocenters was highlighted by the selection of the PIA3 MesoNET project, aimed at pooling computing and training resources and optimizing the Tier1/Tier2 relationship. GENCI has become a member of the SYSTEMATIC competitiveness cluster.

AT THE LEVEL OF THE CIVIL SOCIETY

2020 was, despite the difficult circumstances, a hugely creative year: A Social and Economic Committee (CSE), a travel and visit charter, a computer charter as well as an initial mandatory document covering risk management within the organization. There have also been further job creations.

GENCI has been a major player in the fight against COVID19 and together with the three national centers has been involved since March in nearly 40 projects: understanding the virus, development of target molecules for drug use, simulation for vaccine definition and epidemiological propagation modelling. ■■■

GENCI and the COVID-19 health crisis

ADAPTATIONS AND ORGANISATION OF TEAMS

The health safety measures implemented by GENCI to protect the safety and the physical and mental wellbeing of its employees (Article L4121-1 of the French Labour Code) consisted of three key periods.

As of the initial emergency health decisions taken by the Government in mid-March, GENCI implemented the following measures:

- GENCI's offices were closed and access prohibited,
- Business travel inside France (subject to exceptions) and outside France was banned,
- Remote working arrangements were set-up:
 - suspension of supplier orders,
 - GENCI phone lines transferred to two assistants,
 - installation and configuration of computers for all employees,
 - remote access to the GENCI server,
 - provision of work tools: Webex, OVH phone services, videoconference, Renavisio, document sharing tools,
 - virtually daily Codir,
 - online full staff meetings twice a week.

Regular updates on changes to COVID-19 safety measures were provided for employees.

Following the relaxation of lockdown during May, GENCI reopened its offices. A health safety protocol for GENCI was implemented to allow a gradual return to the office of staff: Reminders of Government recommendations, mandatory wearing of masks in all public areas and shared offices, alcohol-based hand-wash dispensers throughout the buildings, supply of masks, etc. The flexible working arrangements were also continued.



Urgent arrangements made by GENCI to organise remote home working for its employees.

As of the end of October and in accordance with Government instructions, home working has been the preferred option for employees. The offices of GENCI are however open for those whose work requires them to be on the premises.

MOBILISATION OF RESOURCES

With the spread of the pandemic, GENCI and the 3 national centers decided in March 2020 to grant priority access to academic and industrial researchers working on COVID-19. These were thus able, in a matter of days, to access the supercomputers of GENCI and receive dedicated support from the support teams at the 3 national centers.

GENCI was also part of a similar initiative at the European level organised by the PRACE infrastructure by making available the Joliot-Curie computer at TGCC and worked with ANR and Agence Innovation Défense (AID) to provide support for projects launched by these agencies.

So far, GENCI's facilities have supported around forty, French and European, COVID-19 research projects, from both academic and commercial sectors (start-ups, large companies). These covered a wide variety of areas ranging from epidemiological modelling, mass screening for candidate molecules, fine molecular modelling of the binding and activation mechanisms of the SARS-Cov2 virus and its variants, the modelling of droplets spray under all conditions (open air, confined spaces, inside vehicles, mask types, etc.), to the use of artificial intelligence to measure the severity of a pulmonary infection by the virus and detection by the sound of the voice for potentially infected individuals. ■

SIMULATION OF SPEECH EXHALATION FLOWS IN THE TRANSMISSION OF COVID-19



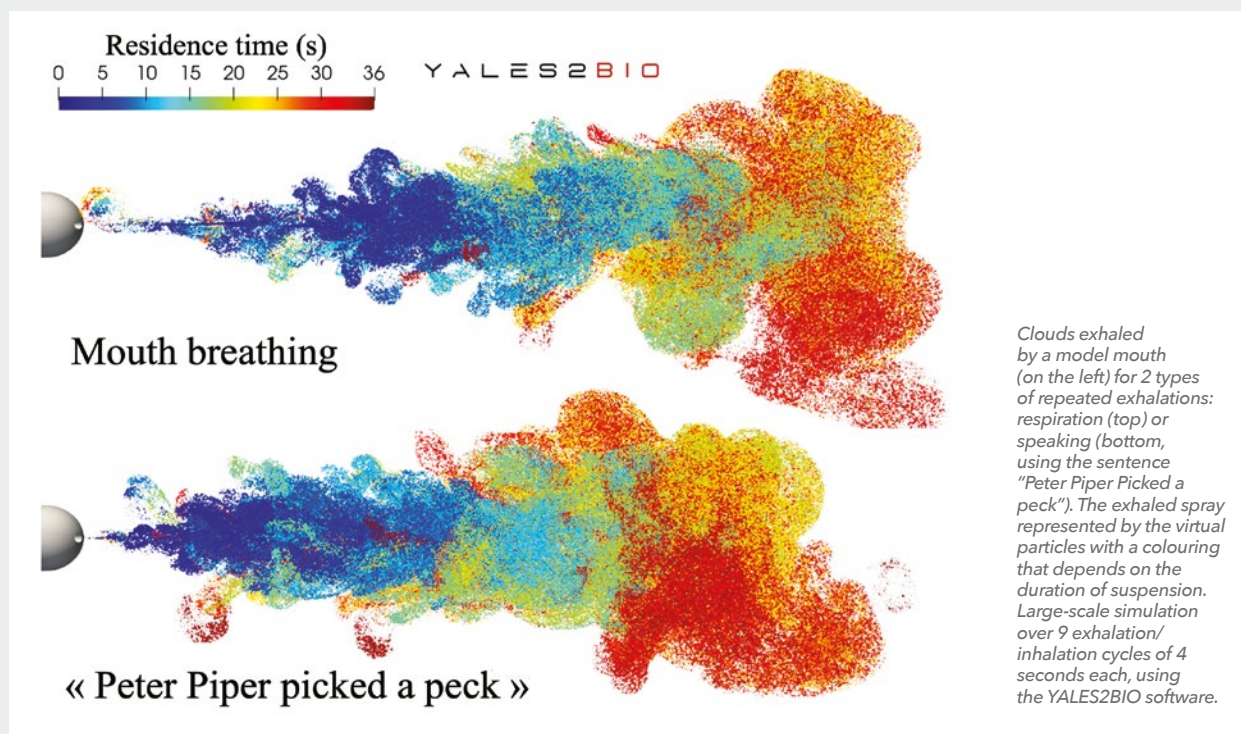
Simon Mendez,
RESEARCHER AT CNRS

Ocigen ⌚ 1.6 million hours

Since 2010, Simon Mendez (CNRS) has been developing the YALES2BIO solver (<https://imag.umontpellier.fr/~yales2bio>), focused on the multiscale simulation of blood flows. Jointly with Franck Nicoud (Professor at the University of Montpellier), he leads the Cardiovascular Biomechanics group at IMAG (UMR 5149, Montpellier). YALES2BIO is based on the massively parallel solver YALES2 (<https://www.coria-cfd.fr/index.php/YALES2>), developed in particular at CORIA (UMR 6614, Rouen) and initiated by Vincent Moureau (CNRS).

The research and computing activity of the YALES2BIO project essentially deals with blood flows, but the events of 2020 led IMAG to start working on the airborne transmission of COVID-19. A major challenge in the management of the COVID-19 crisis is the high level of presymptomatic and asymptomatic transmissions. Such transmissions mainly happen through the droplets of respiratory fluids emitted by non-symptomatic people when they breath, speak or sing, and not just by symptomatic people when coughing or sneezing.

Thanks to allocation A008 from GENCI, IMAG was involved in a study on the flows generated by speech and published in the Proceedings of the National Academy of Sciences in September 2020 (<https://doi.org/10.1073/pnas.2012156117>). This study revealed that certain syllables produce flows that can transport infectious droplets over distances of the order of one meter in a second or less. In addition, the short jets generated during the pronunciation of a succession of words and sentences interact to form a primary turbulent jet that enhances the forward transport of pathogens (see image). This result has been leveraged to propose a model for the space-time risk assessment of short-range transmission of COVID-19 during conversations, published in Physical Review Fluids (<https://doi.org/10.1103/PhysRevFluids.5.122501>).



HIGH-RESOLUTION MOLECULAR DYNAMICS SIMULATION OF SARS-COV-2 PROTEINS

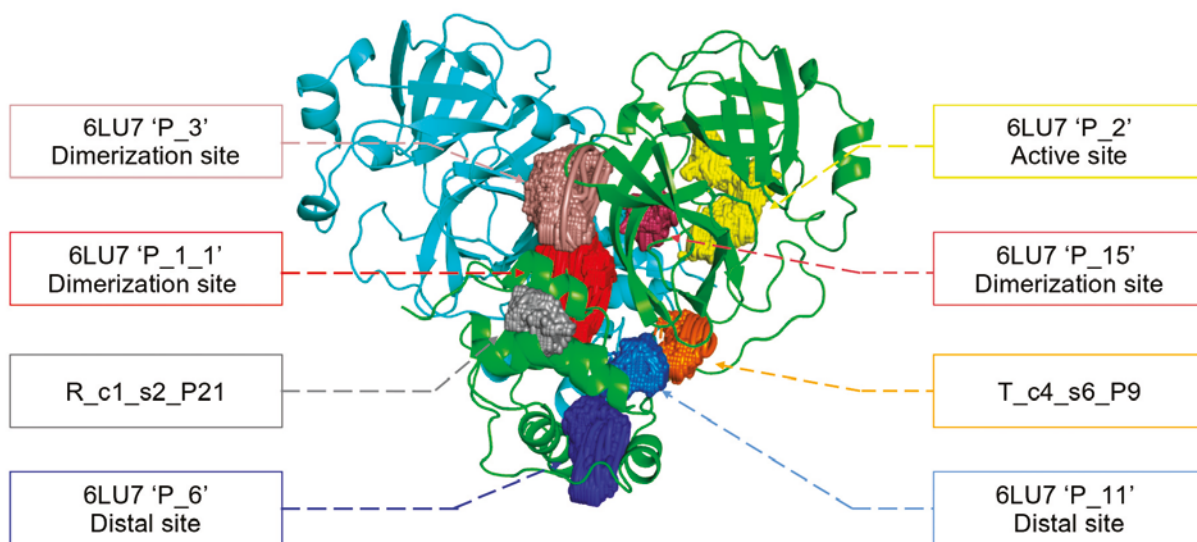


Jean-Philip Piquemal,
DIRECTOR OF THE
THEORETICAL CHEMISTRY
LABORATORY (LCT),
UMR 7616, SU/CNRS

Jean Zay and Joliot-Curie ⌚ 200,000 hours

Started at the end of March 2020, the Tinker-HP project used the resources allocated by GENCI and PRACE (approximately 200,000 GPU hours, 2 million CPU hours, 65% use on Jean Zay, IDRIS, 35% on Joliot Curie, TGCC). The work resulted in:

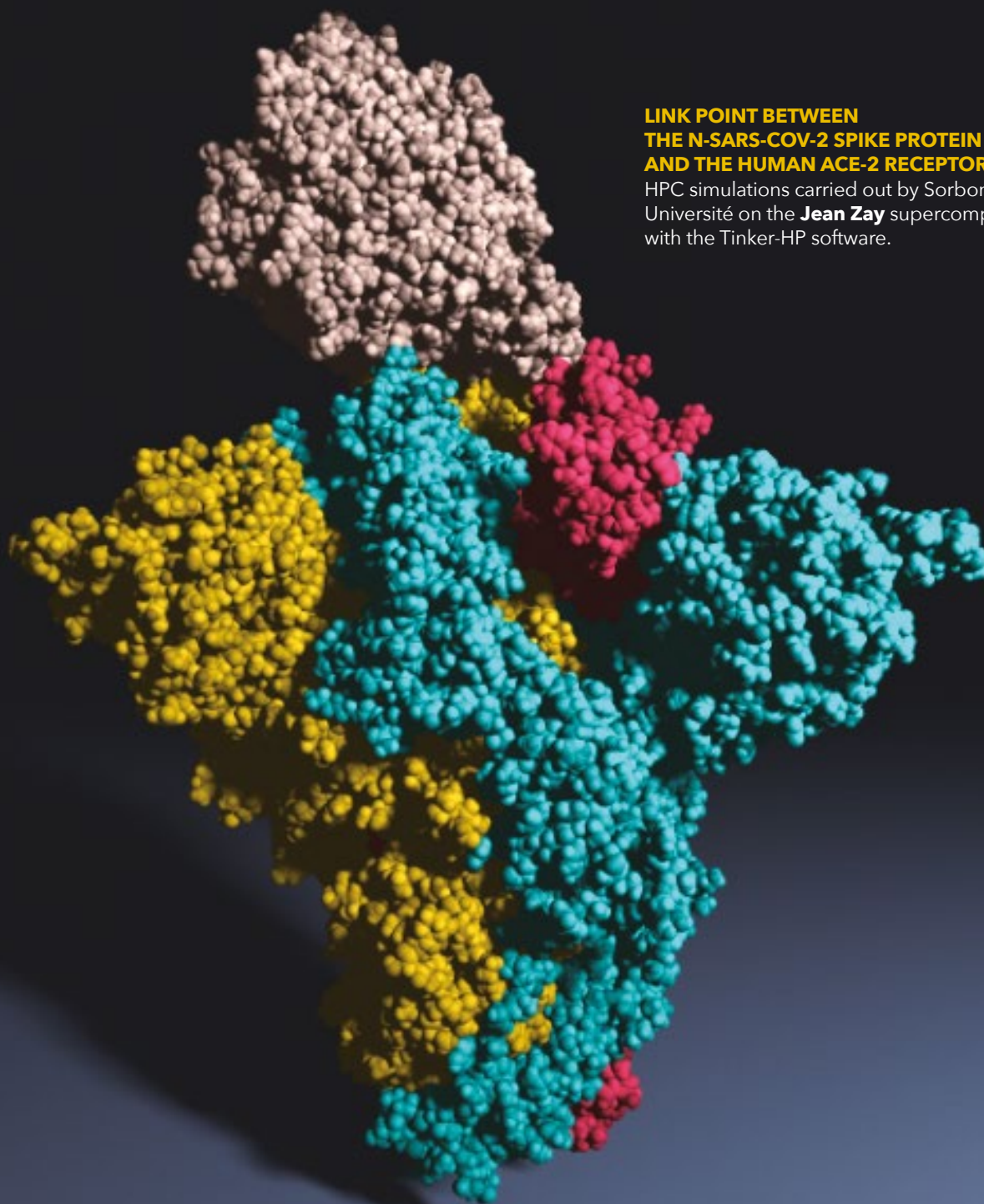
- The production of a multi-GPU (mixed precision) version of the Tinker-HP molecular dynamics software. This was needed to make the very long high-resolution simulations using polarizable force fields possible. A joint publication with IDRIS is available^[1]. The Tinker-HP software is freely available on GitHub^[2].
- The implementation of a new massive adaptive sampling algorithm for molecular dynamics to simultaneously use as many GPUs as available, i.e. between 100 and 1,000 GPUs on Jean Zay (100 on Joliot Curie). A total simulation of nearly 40 microseconds (the largest polarizable simulation ever published) was produced for the SARS-CoV-2 virus Main Protease (Mpro) and analyzed in detail in a recent publication^[3]. This work has established the world's most accurate/extended map of the protein's conformational space (including solvent) and has led to the discovery of potential new docking sites for molecules active against the virus. At the end of 2020, this work, still in progress, continues on other protein targets (Spike protein, papain protease, etc.) working with the experimental teams.



Representation of the enzymatic pocket locations on the SARS-CoV-2 main protease structure.

REFERENCES

- [1] Tinker-HP: Accelerating Molecular Dynamics Simulations of Large Complex Systems with Advanced Point Dipole Polarizable Force Fields using GPUs and Multi-GPUs systems. O. Adjoua, L. Lagardère, L.-H. Jolly, Arnaud Durocher, Z. Wang, T. Very, I. Dupays, T. Jaffrelot Inizan, F. Célerse, P. Ren, J. Ponder, J.-P. Piquemal, J. Chem. Theory. Comput., 2021, online, DOI: 10.1021/acs.jctc.0c01164
- [2] The Tinker-HP software (GPUs) is available on Github: <https://github.com/TinkerTools/tinker-hp/tree/master/GPU>
- [3] High-Resolution Mining of SARS-CoV-2 Main Protease Conformational Space: Supercomputer-Driven Unsupervised Adaptive Sampling. Theo Jaffrelot Inizan, Frédéric Célerse, Olivier Adjoua, Dina El Ahdab, Luc-Henry Jolly, Chengwen Liu, Pengyu Ren, Matthieu Montes, Nathalie Lagarde, Louis Lagardère, Pierre Monmarché, Jean-Philip Piquemal, Chem. Sci., 2021, online, DOI: 10.1039/D1SC00145K



**LINK POINT BETWEEN
THE N-SARS-COV-2 SPIKE PROTEIN
AND THE HUMAN ACE-2 RECEPTOR.**

HPC simulations carried out by Sorbonne Université on the **Jean Zay** supercomputer with the Tinker-HP software.

What the computing centers have to say

The national computing resources, made available to the scientific communities by GENCI, are hosted and operated in three centers: at CPU CINES (Centre Informatique National de l'Enseignement Supérieur), CNRS IDRIS (Institut du Développement et des Ressources en Informatique Scientifique), and CEA TGCC (Très Grand Centre de Calcul).

TGCC, Joliot-Curie



Christine Ménaché
HEAD OF TGCC
(CEA CENTRE HOSTING THE JOLIOT-CURIE SUPERCOMPUTER)



2020 was of course the year that saw the arrival of Covid-19... In addition to managing the teams that had to be very quickly adapted for the successive health constraints during the year, TGCC was asked to provide resources for European and French researchers in the fight against Covid-19, as requested by PRACE and GENCI. Thus, from March 2020 onwards, fifteen new projects were granted access to Joliot-Curie under the “special COVID” program, for a total allocation of around 200 million hours. The related simulations made it possible, for example: to understand the mechanisms of the viral infection, to identify and improve virus inhibitors, to model the dynamics of the propagation of micro-droplets and aerosols, etc. At the same time, the life of the computing center continued, supporting and following up the 24 Grand Challenges (~600 Mh) which ran on the Joliot-Curie “Rome partition” from January to September 2020. All these Grand Challenges were completed and consumed all their allocated computing time.

The acquisition of a new Joliot-Curie partition, Fujitsu ARM A64FX based, was validated by GENCI at the end of 2020, supporting French and European scientists on the path to Exascale. The TGCC teams are getting prepared for this oncoming extension by anticipating the integration of this new partition into the “OCEAN” administration environment developed by CEA/DIF/DSSI. 2021 is already shaping up to be a busy one...

Around fifteen new projects involving approximately 200 million hours of emergency allocation computing time under the “Special COVID” programme.



CINES, Occigen



Boris Dintrans
DIRECTOR OF CINES
(CPU CENTRE HOSTING THE OCCIGEN SUPERCOMPUTER)

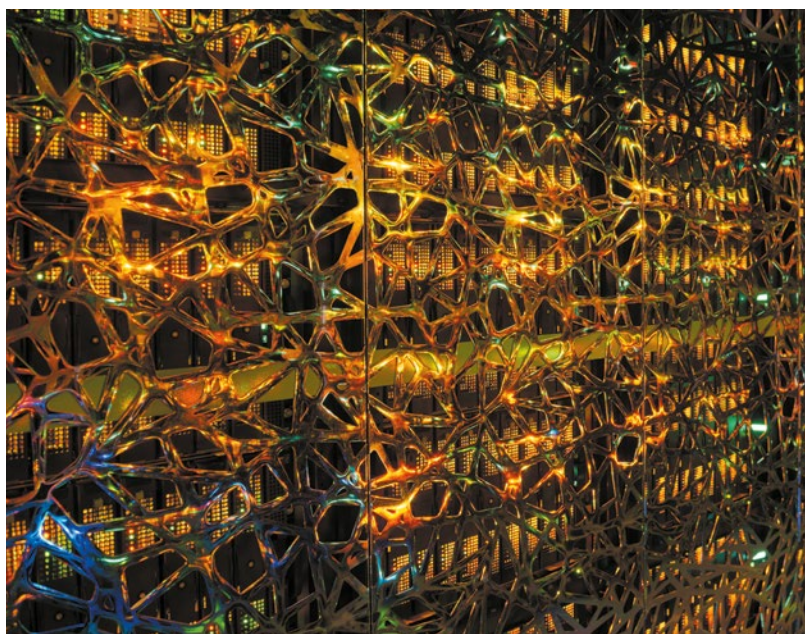


2020: THE YEAR FOR A REPLACEMENT FOR OCCIGEN AND THE YEAR OF COVID-19

620 million computing hours were used in 2020 on the Occigen supercomputer, with an utilisation ratio of 84% for a computer in its 6th year of production. There was a sharp increase in CT5 projects (Theoretical physics and plasma physics) over the last 2 years for Occigen, with 100 million hours now used and a second place on the subjects podium (with CFD once again in 1st place and astronomy/geophysics in 3rd).

Occigen is however reaching the end of its life and in 2020 together with GENCI we initiated its replacement, with the aim of installing its successor in the 1st half of 2022. The new computer will mark a pivotal moment both for the computing teams at CINES and its users, as it will have an accelerated partition which is the only way of delivering the large computing capacity and mastering electricity consumption. Together with this introduction of accelerated computing at CINES, we will be providing specific support for researchers who are often wary of this shift “to GPU”, and it is by working together that we will succeed with the exciting challenge the new computer represents.

2020 was obviously also the year of COVID-19 and CINES played its part, alongside



Together with GENCI we initiated the replacement of Occigen, with the aim of installing its successor in the 1st half of 2022.

GENCI and the CPU, by opening Occigen in urgent computing mode for research projects. 17 million computing hours were used for this urgent computing, with dedicated support for each project, and with HPC once again demonstrating throughout this health crisis its significance for the research community, as well as its effectiveness as a decision making tool.

IDRIS, Jean Zay



Pierre-François Lavallée
DIRECTOR OF IDRIS
(CNRS CENTRE HOSTING THE JEAN ZAY SUPERCOMPUTER)



EXTENSION OF JEAN ZAY TO SERVE THE HPC AND AI COMMUNITIES

In spite of the health crisis and as a result of the continuity of services delivered by the center's teams, IDRIS has been able to complete several major projects, the majority of which were initiated by Denis Girou during his two terms as director.

Among these there was the official inauguration of Jean Zay in January, its extension to 28 Pfllop/s installed in the spring and opened, in July, to the 'Grands Challenges' projects, the finalization of the call for tenders for level 3 storage, support for the AI community (cre-

ation of a dedicated support team) and the rapid acceptance of this national platform with 400 Dynamic Access projects.

In recognition of its dedication, IDRIS was awarded the CNRS Collective Cristal Medal 2020 for the Jean Zay project. Finally, the FITS project (CC-IN2P3/IDRIS collaboration) was selected by an international jury within the framework of the AMI Equipex+ to build a data lifecycle management platform (storage and services) for the IR/TGIR.

IDRIS was awarded the CNRS Collective Cristal Medal 2020 for the Jean Zay project.



“Where are the women?”

With us! In positions of responsibility as project managers for Europe, industrial partnerships, quantum projects, but also: communications, institutional relations, finance and legal affairs. GENCI is thus working to ensure that women are present in numbers in all professional sectors and at all levels.

Would women scientists be more ready to cross the boundaries of disciplinary silos, as illustrated by the following observation: Within the AI support team of CNRS-IDRIS, and beyond, there is significant increase in the numbers of female engineers and researchers in the innovative and transdisciplinary field par excellence which is that of artificial intelligence and the quantum. ■

FIND AND SHARE ONLINE:

Message from Mariya Gabriel during the International Day of Women and Girls in Science / European Commission

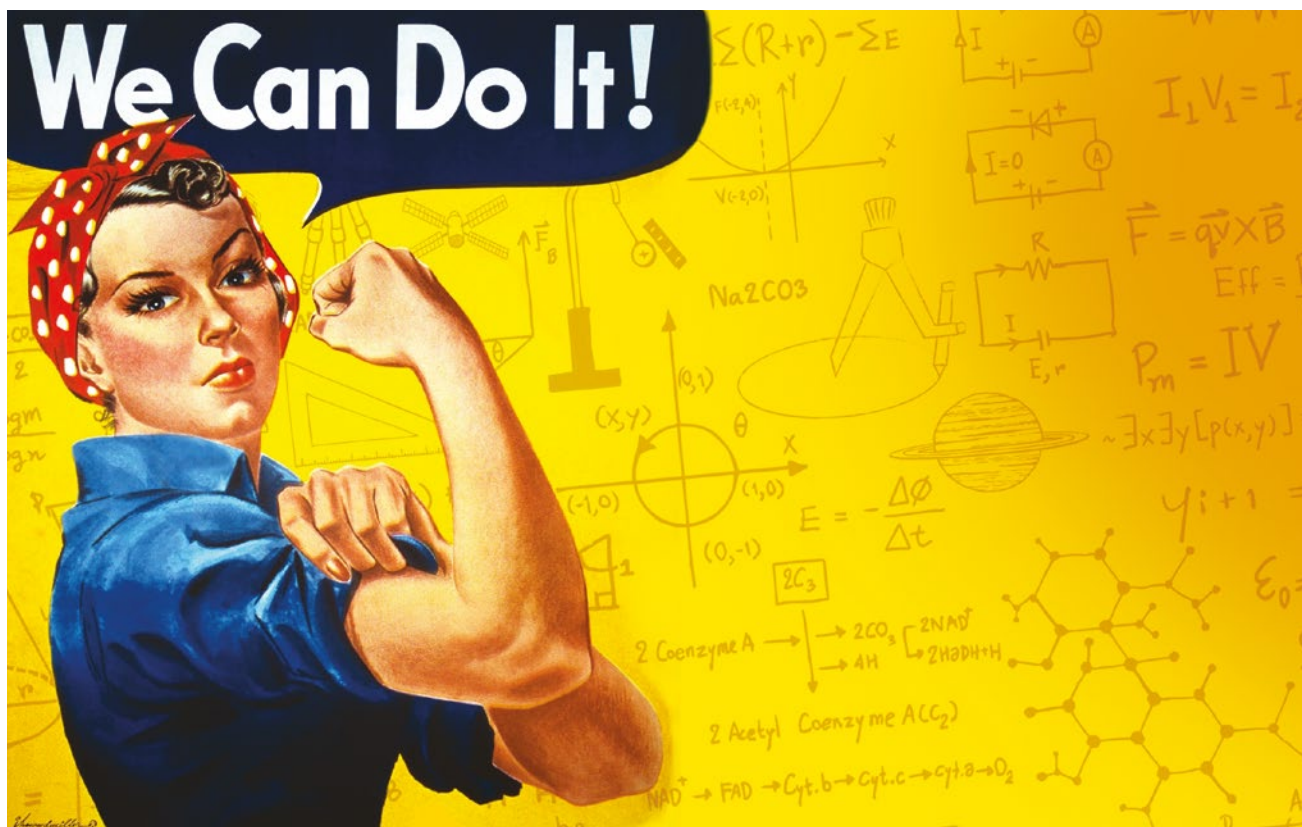


<https://audiovisual.ec.europa.eu/en/video/I-201983>

Ada Lovelace 2021 Prize awarded by PRACE to Dr Céline Merlet

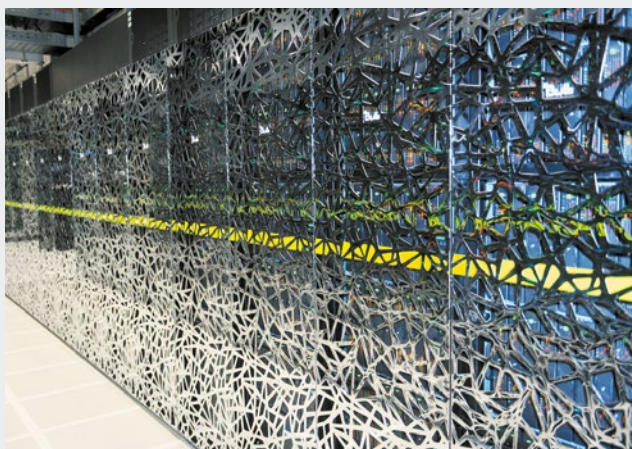
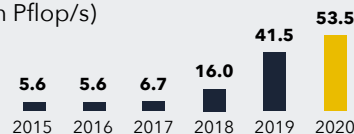


<https://prace-ri.eu/dr-celine-merlet-wins-the-2021-prace-ada-lovelace-award-for-hpc/>



Supercomputers evolution

Growth in computing capacity
(in Pflop/s)



OCCIGEN

BULL BULLX SUPERCOMPUTER **3.5 PFLOP/S**

CINES is hosting an Atos computer with a peak capacity of **3.5 Pflop/s**. With **3,366 nodes** and a total of **85,824 cores**, with 2 Intel Haswell and Broadwell partitions.



JOLIOT-CURIE

ATOS SEQUANA X1000/XH2000 **23 PFLOP/S** SUPERCOMPUTER

TGCC operates an Atos computer with a peak capacity of 23 Pflop/s, composed of **4 partitions**: 3 scalar and 1 for pre/post processing based on a NVIDIA GPU.

A first, scalar, partition with **2,292 AMD Rome based nodes** with **12.7 Pflop/s** and **293,376 cores**.

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

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

A fourth, accelerated, partition of **32 NVIDIA V100 based nodes** for **1.2 Pflop/s** and **128 GPU**.



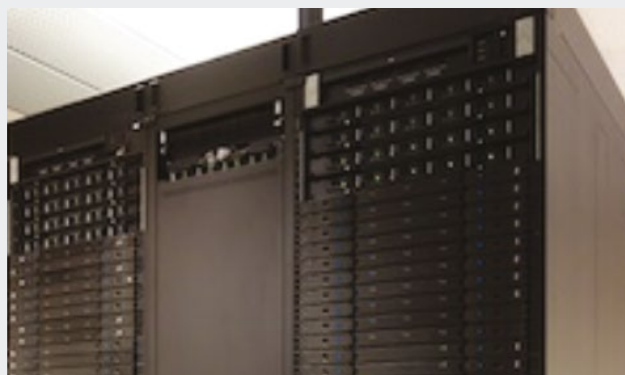
JEAN ZAY

28 PFLOP/S HPE SGI 8600 SUPERCOMPUTER

IDRIS operates an HPE computer with a peak capacity of **28 Pflop/s** and consisting of a scalar partition and a converged partition with a total of **86,344 CPU** and **2,696 GPU**.

A scalar partition of **4.9 Pflop/s** based on **1,528 nodes** with Intel Cascade Lake processors.

An accelerated partition of **23.1 Pflop/s** based on **643 accelerated nodes** and **2,696 NVIDIA V100 GPU**.



OCRE/INTI PROTOTYPE

TGCC also has an Atos prototype, with **30 nodes** based on an Arm Marvell ThunderX2 processor with **1,920 cores**.

The Technology Watch Unit

In 2020, the Technology Watch Unit diversified its computing resources and helped users to develop a better understanding of future HPC and AI technological solutions.

Thus, AMD is donating an 80 hybrid node cluster (640 AMD MI50 GPUs) to GENCI and Inria to pursue and accelerate work against COVID-19 and help users to understand the new ecosystem. Integrated into Grid5000, it will be available mid-2021. Alongside this, the CVT organized 2 hackathons: One, with LEGI (Grenoble INP) and Coria, brought together 50 scientists from the CFD community to migrate and optimize YALES2 and AVBP codes on the AMD processors on Joliot-Curie (TGCC); the other enabled 15

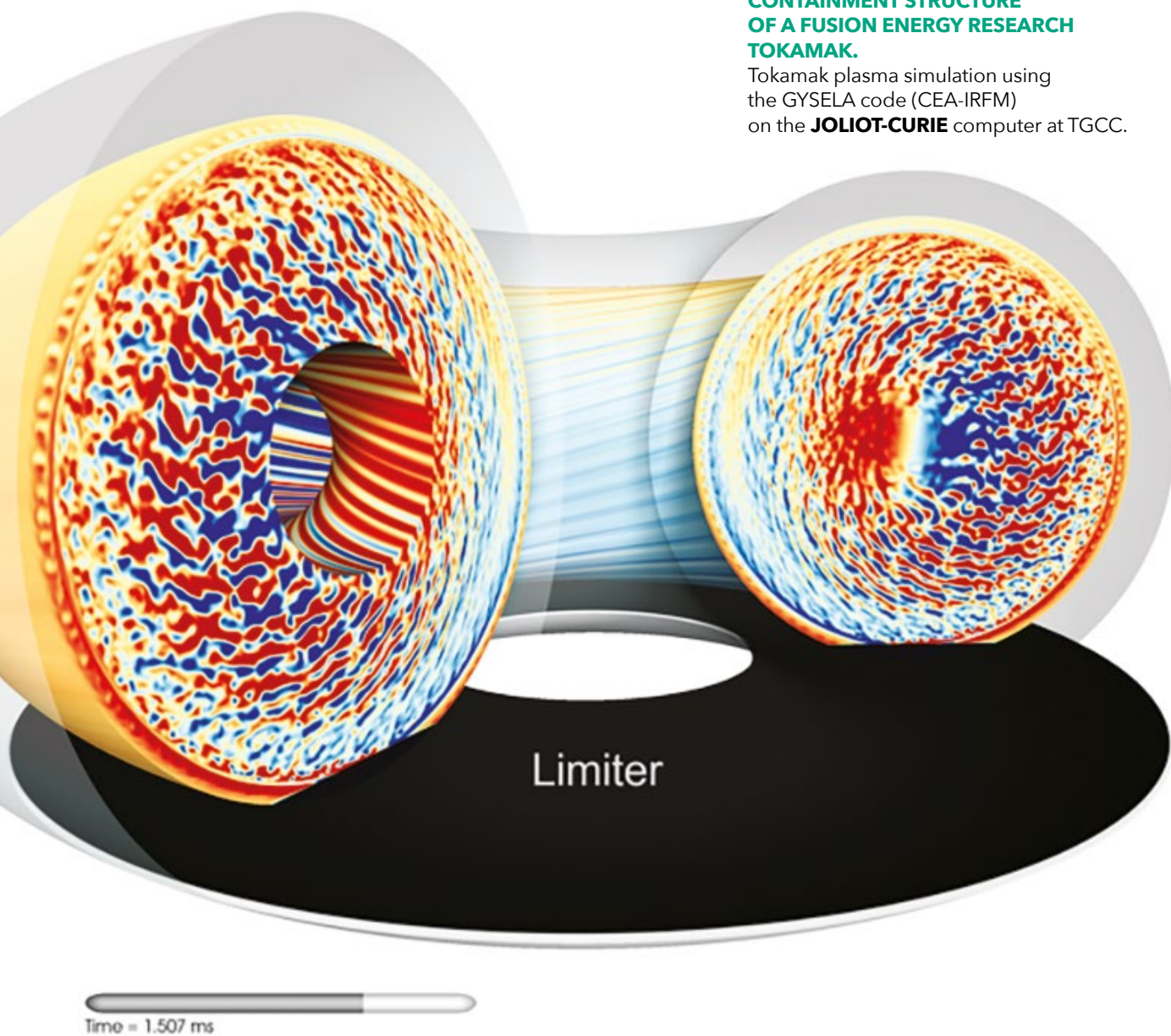
researchers to assess the value of an Arm processor natively supporting vectorization, participate in the co-design of the European EPI processor and thus consolidate the acquisition of a Fujitsu cluster equipped with 80 A64FX SVE native (+ HBM) nodes which will be integrated into Joliot-Curie with access for CVT users mid-2021. ■

ECFD3 PARTICIPANTS:
INDUSTRIAL AND
ACADEMIC RESEARCHERS
WORK TOGETHER IN
DEVELOPING CODES.



**CONTAINMENT STRUCTURE
OF A FUSION ENERGY RESEARCH
TOKAMAK.**

Tokamak plasma simulation using
the GYSELA code (CEA-IRFM)
on the **JOLIOT-CURIE** computer at TGCC.



Academic research results

- 23** Foreword by the Chair of the Evaluation Committee
- 24** Forewords by the Chairs of the Thematic Committees
- 26** 2020 Main scientific results
- 38** DARI - resources available for academic and industrial research
- 39** How to apply for computing time



The work continues despite the health crisis

BY SYLVIE JOUSSAUME, CHAIR OF GENCI'S EVALUATION COMMITTEE

Despite the unprecedented conditions during 2020, because of COVID-19, operations at the national computing centers continued as normal. Thanks go to all the staff of these computing centers! The Thematic Committees were also able to provide their expertise and, like everyone else, we all switched to the world of the videoconference.

A high level of pressure continued for the DARI A8 and A9 applications, in particular on the Joliot-Curie SKL, Occigen and Jean Zay CSL computers. The start of production using the Rome partition on Joliot-Curie and the transfers of projects between computers and partitions ensured we could best meet the requirements of the various communities. The degree of solidarity between the Thematic Committees and the cooperation between the computing centers once again proved a winning formula, ensuring the optimum use of the available resources. Huge thanks are due to the project leaders who agreed to these transfers!

2020 was also marked by the CINES call for tenders, ongoing, and which will help boost computing resources in 2022. Over

the year the Thematic Committees have been involved in the consideration of changes to the process for allocating computing resources and in particular the possibility of relaxing the rules for small projects. This examination will continue in 2021, the year in which, more than ever, we are going to have to get ready to use accelerated computers to be able to benefit from the arrival of the European pre-exascale computers! ■

“The degree of solidarity between the Thematic Committees and the cooperation between the computing centers once again proved a winning formula, ensuring the optimum use of the available resources.”

Forewords by the Chairs of the Thematic Committees



**CT1
ENVIRONMENT**
GERHARD KRINNER
Chair of CT1

The research areas covered by CT1 Environment include a wide range of themes, approaches, spatial and temporal scales, from the climate of Jupiter to atmospheric flows in a windfarm, the Earth's climate from millions of years ago to that of the next century. This year, once again, we have had the pleasure of seeing outstanding modelling results, made possible thanks to the excellent availability of GENCI's computers, despite these truly unprecedented conditions. Thank-you!



**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 72 projects this year highlight this diversity, by helping to increase our understanding of turbulent flows and of the associated hydrodynamic instabilities for applications at the heart of today's key challenges: energy conversion, environment, processes, etc.



**CT2B
REACTIVE AND
MULTIPHASE FLOWS**
PASCALE DOMINGO
Chair of CT2b

In 2020, 42 projects, including 10 new projects, submitted to CT2b were

allocated CPU time on GENCI's supercomputers. The range of the research topics addressed by CT2b is extremely wide, as it includes all flows that are reactive and/or diphasic. The projects are related to upstream research, as well as close to application research, covering fields such as energy production and use, environmental problems, production of nanoparticles, dispersion of pathogenic agents, etc. Most of the software are non-commercial, producing extremely good results whatever the computer architecture. Although GPU architectures are not yet widely used, developments are currently underway to migrate certain codes, with support from the computing center teams.



**CT3
BIOLOGY AND HEALTH**
LAURENT DESBAT
Chair of CT3

"CT3" (Biology and Health) evaluated 7 projects in A8 and 4 in A9, including 3 new projects, for a global allocated computing time (in Mh): Jean Zay CPU 7.8 and GPU 0.01, Occigen 8, Joliot Curie SKL 2, KNL 0.5, Rome 13. The projects cover immunology, genetics, molecular dynamics, antibodies and antigens, fluid dynamics, cardiac electrical activity, brain imaging, etc.



**CT4
GEOPHYSICS AND
ASTROPHYSICS**
FRÉDÉRIC BOURNAUD
Chair of CT4

LCT4 in astrophysics and geophysics saw a roughly constant number of projects,

but the number of very large projects requiring several millions of core hours on several GENCI supercomputers continues to grow.

In particular, there is a growing number of large projects in cosmology, associated with the arrival within the next months and years of data from new large ground-based and space observatories.



**CT5
THEORETICAL PHYSICS
AND PLASMA PHYSICS**
ÉRIC SERRE
Chair of CT5

38 high-level projects covering a wide spectrum of fundamental physics shared more than 20% of the total available resources this year. Quantum chromodynamics, magnetic confinement fusion, and high-intensity lasers nonetheless continue to account for 90% of the hours.

There was further confirmation of the emergence of projects based totally or partially on new processor architectures (7 XeonPhi and GPU projects). In particular, we witnessed the successful migration of codes from QCD to GPU.



**CT6
COMPUTING,
ALGORITHMES AND
MATHEMATICS**
DIDIER AUROUX
Chair of CT6

CT6 evaluated around 15 projects in 2020, in line with previous years.

These cover a wide range of topics from numerical algorithms to parallelization problems (resolution of large linear

systems, development of libraries, scalability). At the interface between HPC and AI, some projects focused on the construction of reduced models, requiring very many hours to build a database of numerical simulations in different configurations.



CT7
MOLECULAR MODELLING APPLIED TO BIOLOGY
PATRICK FUCHS
Chair of CT7

As in 2019, CT7 evaluated around thirty applications per call in 2020. Approximately 100 million CPU hours were allocated along with one to two million GPU hours. Our community continues to be an active user of GENCI GPU resources. In fact, in 2020 we were one of the biggest consumers. Our activity deals with the modeling of biological molecules such as proteins, nucleic acids, lipids, carbohydrates, small molecules, etc. Molecular dynamics (MD) is a central concern here. MD allows the simulation of the movements and interactions of these biomolecules with their environment or with each other. A growing number of projects include, for example, membrane proteins in interaction with their lipid membrane and the aqueous solvent on either side of the membrane.

In addition, so-called augmented sampling methods are increasingly used. They allow the study of slow phenomena at the molecular scale, such as the passage of molecules through a membrane, ligand binding to a protein and many more. The resources of GENCI are essential in carrying out this work, which uses MD engines capable of operating in a massively parallel manner.



CT8
QUANTUM CHEMISTRY AND MOLECULAR MODELLING
DAVID LOFFREDA
Chair of CT8

During 2020 and in the difficult context of the COVID-19 health crisis, theoretical modeling in quantum chemistry has shown more than ever its importance in understanding chemical bonding, with many applications covering the fields of chemistry, physics and of course biology.

The studied systems are increasingly complex in describing electronic interactions and realistic with respect to experiment, especially with the emergence of reactive interfaces, which play a fundamental role in many fields, including in biomedical research. This has resulted in a further increase in the computing resources requested this year, in a strong context of telecommuting, where permanent access to GENCI's computing resources has been crucial.

The community of CT8 researchers, consisting of developers, code contributors and users, continued to interact with the application supports of the three GENCI centers, in particular for installing all the quantum chemistry codes on the new machines: Jean Zay V100 GPU at IDRIS and Irene V100 GPU at TGCC. The committee therefore offers its thanks to them once again for their technical support.



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

The number of applications continues to rise and reached 119 allocation requests (56 in the A8 session in February and 63 for A9 in September 2020), with a

proportion of new projects of around 30%, a sign of the health of the community. With the emergence of machine learning, complex workflow simulations are beginning to appear. The use of graphic accelerators continues to expand. A huge range of problems are being examined and require computing power in the hundreds of Teraflops a second at a maximum, but with very many jobs run in parallel or subsequently.

One area that is not being currently processed using the GENCI computers is the analysis of experimental data, the volumes of which have increased very significantly in recent years at a magnitude of several Tb per experiment. The analysis of these data, in particular for 3D reconstructions of the structure of materials, leads to the generation of workflows mixing experimental data, atomic scale simulations, such as molecular dynamics, and machine learning for mapping defects or structures.

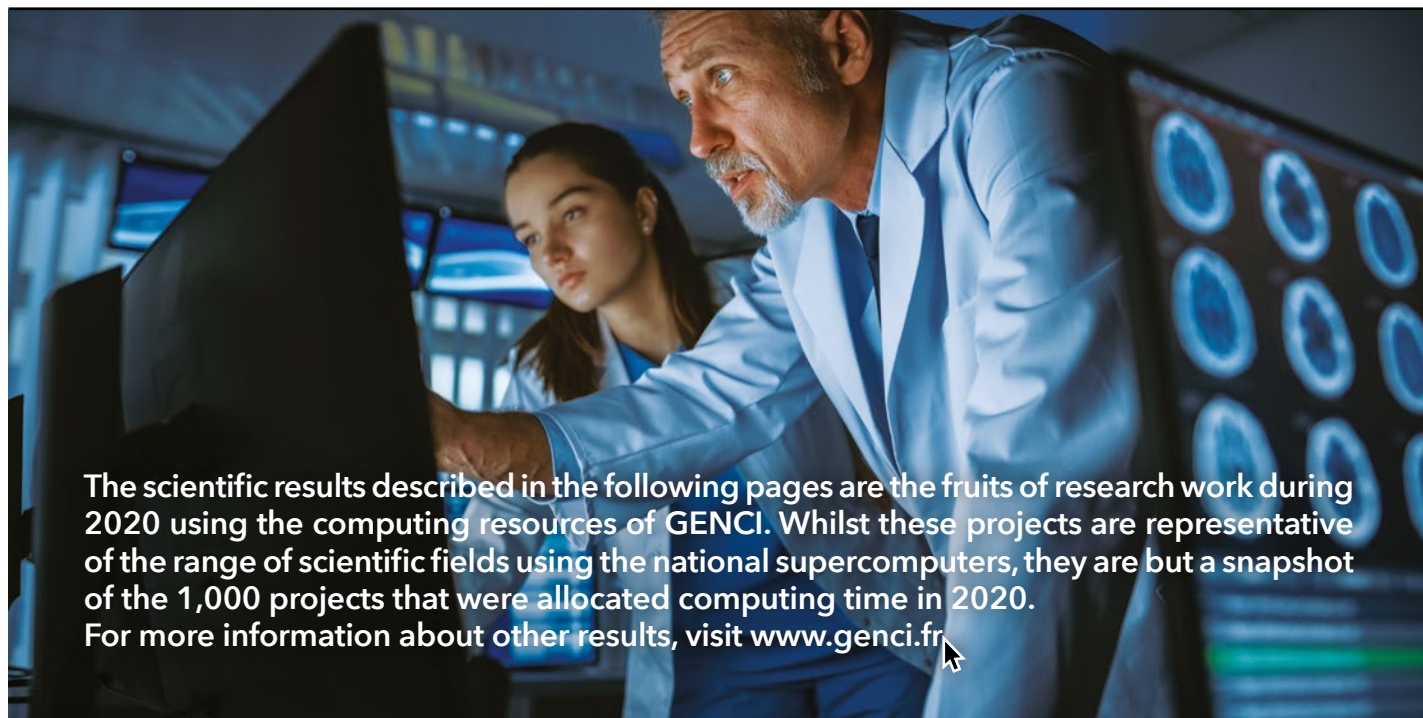
This trend makes real the convergence between HPC, HPDA (High Performance Data Analytics) and artificial intelligence.



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

CT10 reviewed 13 proposals, for a total allocation of 60 million hours.

Many proposals were concerned with the transversal fields of nuclear reactors, planet mineralogy and electromagnetism. The enlargement of the CT to Artificial Intelligence also resulted in 5 excellent proposals (autonomous agents, task or word learning, histology), together with the success of the dedicated portal.



The scientific results described in the following pages are the fruits of research work during 2020 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 1,000 projects that were allocated computing time in 2020. For more information about other results, visit www.genci.fr

2020 main scientific results

27 Theoretical physics

CT5: Understanding the abnormal transport of electrons in the magnetised cold plasmas used for satellites electric propulsion systems

28 Earth and universe sciences

CT1: Chemical composition of the atmosphere and population exposure

CT4: Throwing light on the magnetosphere of black holes

30 Fluid mechanics

CT2a: Understanding quantum turbulence on all scales

CT2b: Non-equilibrium thermochemical hypersonic turbulent flows

32 Biology, chemistry and materials

CT9: Advanced protein/protein or protein/ligand binding energy estimator based on electronic structure coupled with molecular dynamics

CT8: Quantum modelling decodes catalysers

CT7: The Hamlet curse of a protein: to be or not to be stabilized by the crowd

35 Other applications (computing, health, etc.)

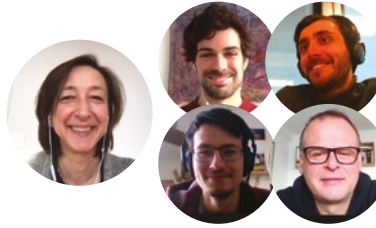
CT3: Predicting blood flows in intracranial aneurysms after treatment

CT6: Improving the competitiveness of the HPC software stack

CT10: DeepCuriosity: Exploration guided by curiosity and developmental learning in AI

CT5 THEORETICAL PHYSICS
AND PLASMA PHYSICS

Occigen ⌚ 12 million hours



Anne Bourdon,
DIRECTOR OF RESEARCH CNRS,
PLASMA PHYSICS LABORATORY,
UMR7648

**Alejandro Alvarez, Federico Petronio,
Thomas Charoy, Pascal Chabert**

Theoretical physics

Understanding the abnormal transport of electrons in the magnetised cold plasmas used for satellites electric propulsion systems

Plasma Physics Laboratory - Ecole Polytechnique

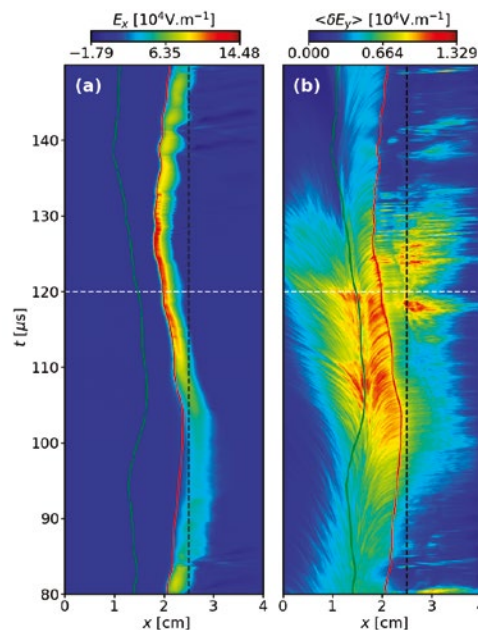
In recent years, electric propulsion is increasingly used for full orbit raising and station keeping of satellites and propulsion of space probes. Of the various electric propulsion systems, the most efficient are the Hall thrusters developed by SAFRAN Aircraft Engines, the industrial partner of the POSEIDON Chair at LPP with the Agence Nationale de la Recherche. Hall thrusters have been extensively studied since their invention in the 1960s.

However, the physics of magnetized plasmas typical of these thrusters is complex; several plasma processes that have direct relevance to the thruster performance and lifetime are still poorly understood (plasma instabilities, wall erosion, etc.). Today, the design and development of Hall Thrusters is still semi-empirical with long and expensive live tests. A better knowledge of low-temperature low-pressure magnetized plasmas in these thrusters is necessary both to reduce the number of experimental tests and to provide the foundation for breakthroughs in the designs of new electric thrusters.

At LPP we started developing in 2014 a 2D electrostatic “Particle-In-Cell” code, known as LPPic, specifically for studying plasma instabilities and their impact

on the increase of the electron transport, called “anomalous transport” in the literature. With the computing hours on OCCIGEN we have, for the first time, carried out an exhaustive parametric study to validate a theoretical model developed recently by our team for the elec-

tron transport. This work is a key step towards the development of new fluid and hybrid models for low-temperature plasmas which will allow the coupling of detailed plasma simulations with experimental tests in developing new electric thrusters. ■



Typical high frequency (100-150 kHz and 2-3 MHz) fluctuations during one low-frequency (10-15 kHz) “breathing mode” oscillation of the Hall thruster. Time and axial (propulsion direction) evolution of: (a) the axial electric field, (b) azimuthal electric field fluctuations. Green vertical line: axial position of null ion axial velocity. Red vertical line: axial position of ion sonic point. Vertical black dashed line: axial position of maximum magnetic field.

CT1 ENVIRONMENT
Joliot-Curie ☉ 50,000 hours



Myrto Valari,
 DEPUTY PHYSICIST (CNPAT) AT
 THE DYNAMIC METEOROLOGICAL
 LABORATORY LMD/IPSL, OSU
 ECCE-TERRA, SORBONNE UNIVERSITÉ

Earth and Universe Sciences

Chemical composition of the atmosphere and population exposure

Chemistry-transport models simulate the spatio-temporal evolution of several atmospheric contaminants present in the air in gas, liquid or solid state. These algorithms simulate the chemical transformations of pollutants as well as their transport and mixing in the atmosphere. The LMD coordinates the development of the CHIMERE chemistry-transport model. The scale of our studies covers a wide range from urban to hemispheric scales. A special focus is on the urban scale, where air-pollution health effects are particularly pronounced. Downscaling methods have been developed to separate the contribution of the various emission sources and to represent the spatial variability of pollutant concentration at fine scale.

However, to quantify the impact of atmospheric pollution on human health by associating pollutant concentrations with health data, the outdoor concentration of the pollutant alone is not enough. One needs to also account for pollutant concentration indoors as well as the time spent by the population at different indoor and outdoor locations. In a recent study we combined pollutant concentrations simulated with CHIMERE over the Ile-de-France region with demographic data, time-activity sequences, as well as with building characteristics that allow the modelling of the transfer of outdoor air-pollution indoors. The first figure is a map (the first to our knowledge) of the Parisian population's exposure to airborne particles with a diameter small-

er than $2.5 \mu\text{m}$ ($\text{PM}_{2.5}$). The spatial distribution of exposure here depends not only on pollutant concentrations but also on the distribution of buildings and human activity. The second figure shows the modelled intra-urban variability in

$\text{PM}_{2.5}$ exposure as a function of the transportation mode. Overall, 20% of the population using bicycles or motorcycles is exposed to annual average $\text{PM}_{2.5}$ concentrations above the EU target value ($25 \mu\text{g}/\text{m}^3$).

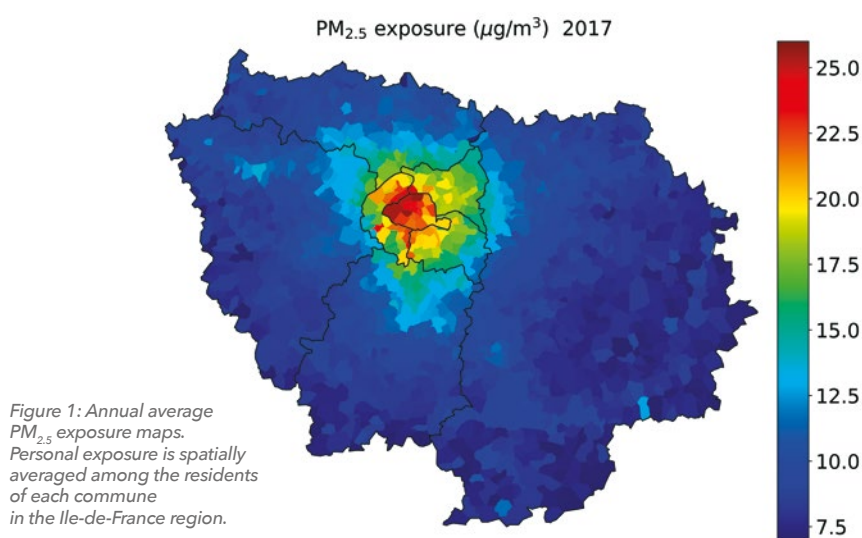


Figure 1: Annual average $\text{PM}_{2.5}$ exposure maps. Personal exposure is spatially averaged among the residents of each commune in the Ile-de-France region.

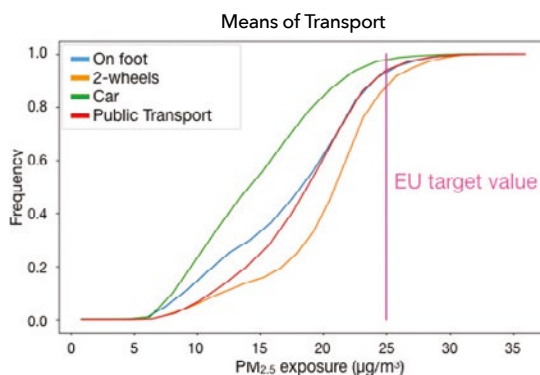


Figure 2: Cumulative distributions of exposure to $\text{PM}_{2.5}$ for sub-populations distinguished by the home-place of work transportation mode in the Ile-de-France region.

CT4 GEOPHYSICS AND ASTROPHYSICS

Occigen ⌚ 1.5 million hours

Joliot-Curie ⌚ 12 million hours



Benoît Cerrutti,
SENIOR
RESEARCHER
AT CNRS



Benjamin Crinquand,
DOCTORAL STUDENT
AT UNIVERSITÉ
GRENOBLE ALPES

Earth and Universe Sciences

Throwing light on the magnetosphere of black holes

Institute for Planetary Sciences and Astrophysics Grenoble, CNRS, Université Grenoble Alpes.

Stellar-mass and supermassive black holes are believed to be the central engine in a wide variety of high-energy cosmic phenomena. Active black holes are often surrounded by a hot disk of gas and dust and a jet of matter launched at the speed of light. This activity is accompanied by a highly efficient acceleration of particles and an intense electromagnetic radiation from radio waves to gamma rays.

Thanks to recent progress in radio and infrared interferometry, it is now possible to very closely observe the event horizon of the nearest supermassive black holes, the image of the shadow of M87* is perhaps the most spectacular demonstration of these new capabilities. The observed signal is most likely synchrotron radiation emitted by relativistic electrons immersed in an intense magnetic field held in place by a plasma orbiting around the black hole. Our work aims at producing the most realistic model of the magnetosphere forming around a rotating black hole, with the ultimate goal of bridging the gap between models and observations. This is a difficult challenge because it couples multiple spatial and temporal scales, and it involves general relativity, plasma physics and quantum electrodynamics. Such a complexity can be captured by particle-in-cell simulations, which model a plasma as a collection of individual par-

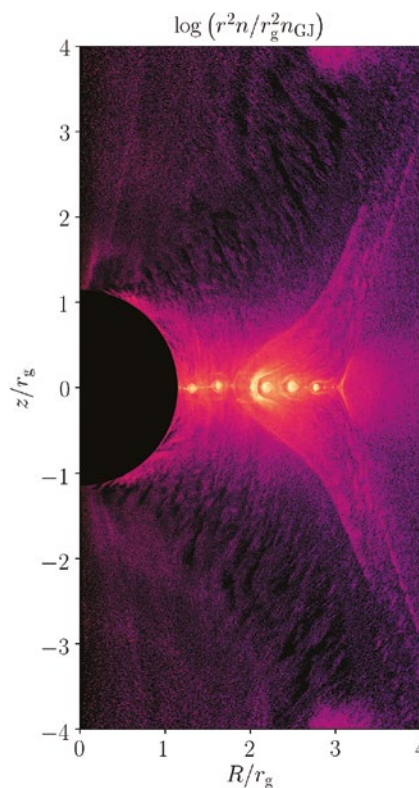


Figure 1: Density map of the plasma of electron/positron pairs created in the vicinity of a rapidly rotating black hole (the black disk shows the event horizon). The simulation was performed with the particle-in-cell Zeltron code on Occigen.

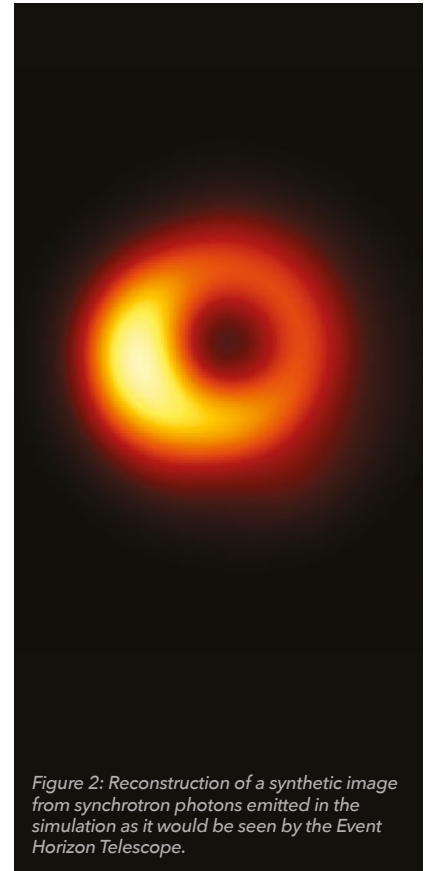


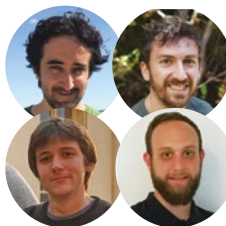
Figure 2: Reconstruction of a synthetic image from synchrotron photons emitted in the simulation as it would be seen by the Event Horizon Telescope.

ticles evolving self-consistently with the electromagnetic fields. Thanks to GENCI resources, we have shed new light on the mechanism of black hole spin extraction by a plasma of electron/positron pairs created in the vicinity of the event hori-

zon. The rapid rearrangement of magnetic field lines leads to efficient particle acceleration and to intense electromagnetic radiation, which could well be at the origin of the enigmatic ring of light seen around M87*.

CT2A NON REACTIVE AND MULTIPHASE FLOWS

Occigen and Joliot-Curie ⌚ 2 million hours



Giorgio Krstulovic,
SENIOR RESEARCHER CNRS
Juan Polanaco, Nicolas Muller,
Umberto Giuriato

Fluid mechanics

Understanding quantum turbulence on all scales

J.L. Lagrange Laboratory CNRS UMR 7293, Université Côte d'Azur, Observatoire de la Côte d'Azur.

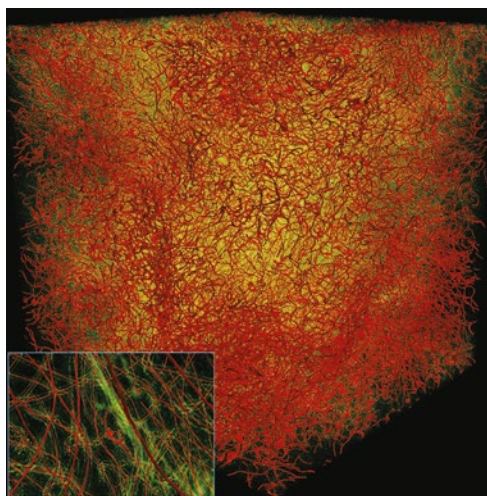


Figure 1

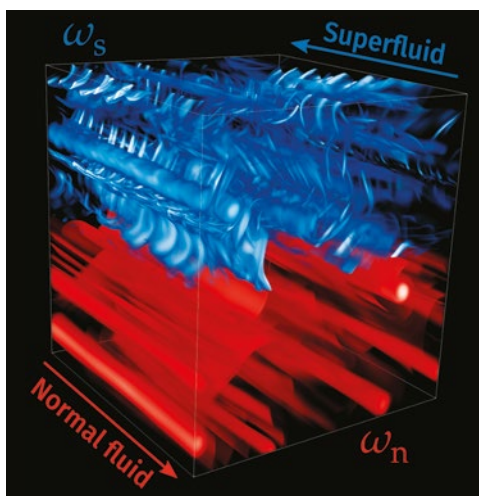


Figure 2

Fig. 1: Numerical simulation of a turbulent superfluid using the Gross-Pitaevskii equation. Vortices correspond to red filaments and density waves are rendered in yellow colours. The inset shows a zoom of the flow. Ref: Phys. Rev. B 102,13 (2020).

Fig. 2: Numerical simulation of counterflow turbulence using the Hall-Vinen-Bekarevich-Khalatnikov (HVBK) model. The figure shows vorticity visualisation exhibiting a quasi-two-dimensional behaviour. Ref: Phys. Rev. Letts. 125, 254504 (2020).

Superfluids are fluids whose behaviour is dictated by quantum mechanics but which at large scales resemble perfect fluids. Remarkably, their viscosity identically vanishes and they contain vortices whose circulation is quantised. One well studied example in the laboratory is helium at temperatures below 2K. To describe it, there are different models to account for the physics at the scale of quantum vortices (Angstroms) or at the scales of turbulence (several centimetres) and in different temperature regimes.

We have performed numerical simulations of a turbulent superfluid at very

low temperatures using the Gross-Pitaevskii model which enables a small-scale physical description, including quantum vortices with quantised circulation. Figure 1 shows a turbulent state made up of thousands of quantum vortices (red filaments) interacting with density waves (in yellow). At large scales, these vortices give rise to a turbulent state with the same properties as a classical fluid. At small scales (inset), individual quantum vortex dynamics predominate, and vortex reconnections and Kelvin waves (waves that propagate along vortices) are responsible for energy transfers.

The study of finite temperature helium at large scale is given by other macroscopic models. We have used the HVBK equations where the flow is described as consisting of two immiscible fluids. This model makes it possible to study a turbulent state where the two fluids have a non-zero relative mean velocity. Such an out-of-equilibrium state, called counterflow turbulence, has no analogue in classical fluids. We have shown that when the counterflow is strong enough, the superfluid transits from a three-dimensional state to a quasi-2D system. Figure 2 shows vorticity visualisations of counterflow superfluid turbulence.

CT2B REACTIVE AND MULTIPHASE FLOWS

Joliot-Curie ☉ 5.5 million hours

Jean Zay ☉ 4 million hours

Occigen ☉ 1 million hours



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Fluid mechanics

Non-equilibrium thermochemical hypersonic turbulent flows

Hypersonic flows are an area of major concern for planetary reentries of space vehicles or high speed atmospheric flight. The very high temperatures reached near surfaces trigger various thermophysical processes, including vibrational excitation, chemical dissociation and gas-surface interactions. These phenomena typically occur on time-scales similar to those of fluid motion, resulting in a thermochemical non-equilibrium (TCNE) state having a serious impact on aerodynamic performances, heat transfer, ablation and growth rates of flow instabilities.

Particularly critical is the occurrence of a turbulent flow regime, leading to severely

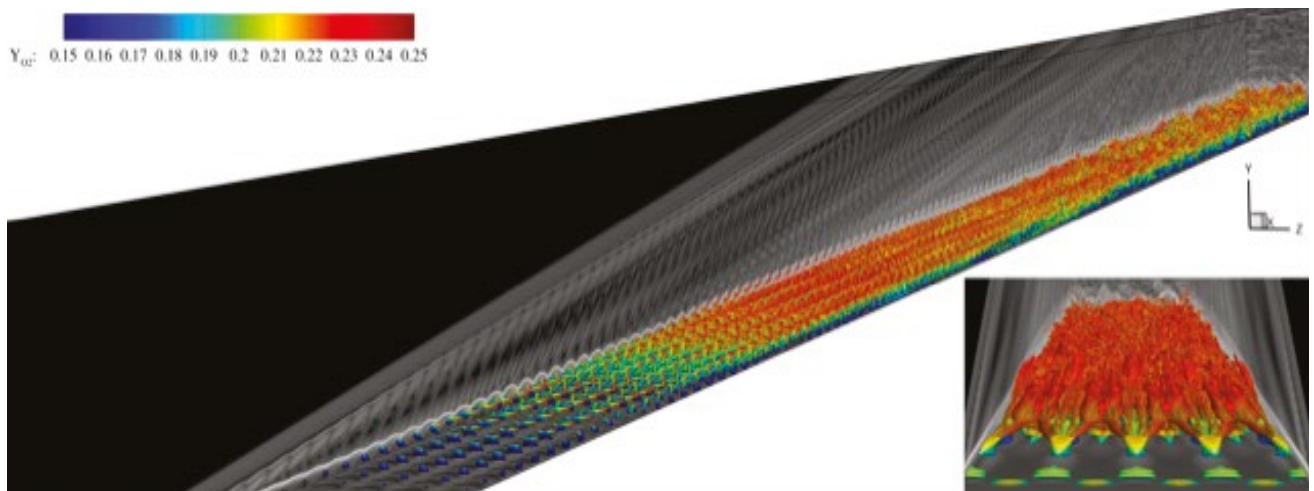
increased wall friction and heat transfer. Existing turbulence models lack accuracy for these applications and carrying out experiments is complex, given the difficulties in reproducing such extreme conditions: high-fidelity numerical simulations are thus essential for improving our fundamental knowledge of such flow mechanisms.

Over the past few years, the DynFluid Laboratory has been developing a HPC code, HPCFD, for numerical simulations of high-speed flows. It relies on very high-order numerical schemes ensuring shock-capturing capabilities, and includes advanced models for multi-species

transport, air dissociation and vibrational relaxation.

The allocation by GENCI enabled the performance of the first-ever direct numerical simulation (DNS) of a hypersonic boundary layer in TCNE, using a domain encompassing the laminar-to-turbulent transition regime discretized with more than 1.5 billion grid points.

This data will provide a valuable reference for the analysis of TCNE-turbulence interactions and the development and calibration of suitable RANS closures, contributing to unraveling the complex behaviours of such flows. ■



DNS of a hypersonic boundary layer in chemical non-equilibrium. The turbulent structures are colored by the local oxygen mass fraction, indicating a strong chemical activity close to the wall. The density gradient magnitude (plotted in grayscale on the lateral planes) reveals the complex pattern of wave propagation outside the boundary layer. At the bottom right, a zoom on the forcing and transitional regions is provided.

CT9 PHYSICS, CHEMISTRY AND MATERIALS PROPERTIES

Joliot-Curie/AMD Rome 🕒 5 million hours



Luigi Genovese,
DIRECTOR OF THE ATOMISTIC
SIMULATION LABORATORY
(MEM/L_SIM), CEA, IRIG

Biology, chemistry and materials

Advanced protein/protein or protein/ligand binding energy estimator based on electronic structure coupled with molecular dynamics

This work is being carried out jointly with Michel Masella (CEA, Institut Joliot-Curie) as part of a project under CT3.

The wavelet-based electronic structure code, BigDFT, enables Density Functional Theory calculations which scale linearly with the number of atoms, in contrast to the traditional approaches which exhibit a cubic scaling behavior. Thanks to its unique features, full Quantum Mechanical descriptions of (solvated) proteins are accessible up to systems of tens of thousands of atoms. Combined with a molecular dynamics code, Polaris, BigDFT has been successfully applied to macro-molecular systems in biology, notably in connection with the COVID pandemic, by making it possible to identify the active fragments of a protein in the presence of a target molecule and to provide the key parameters for their modelling.

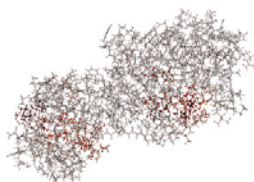
Targeting specific monoclonal antibodies can be routinely achieved, however increasing the antigen affinity as much as desired is still a challenging task. Most of the available theoretical tools in this field mainly focus on investigating close contact antibody/antigen (AA) local regions and usually ignore the effect on affinity of more distant domains. Because of the size of AA assemblies only standard pairwise molecular modeling force fields or empirical cost function are used to quantify the

strength of their interactions. However these theoretical approaches are known to be based on crude approximations making it impossible to achieve a level of accuracy which is sufficiently high.

Our project, the winner of a *SANOFI iTech Award 2020*, adds two new steps to standard computational protocols used to model AA assemblies (for instance the popular one based on the Rosetta package of programs) to further evaluate and

refine their solutions. These two steps involve:

- (1) investigating the AA potential energy surface from “Replica Exchange” molecular dynamics simulations based on a polarizable multi-scale molecular modeling approach;
- (2) refining the simulation results using the complexity reduction framework of BigDFT, enabling the computing of the quantum interaction energy of complete AA assemblies.



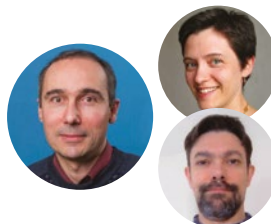
```
field_vals=Interaction_strengths(sys.keys(),fr,pairwise_bo)
colordict=V.get_colordict(keys=sys.keys(),field_vals=field_vals)
#colordict=V.get_colordict(keys=sys.keys(),field_vals=[abs(pv[frag]) for frag in sys])
#colordict=V.get_colordict(keys=sys.keys(),field_vals=[np.linalg.norm(frag.dl()) for frag in sys.values()],colorcode='Greens')
colorletters=colordict[frag] for frag in rl)
plot_sequence(sq[0]+sq[1],colors=colorletters)
```

S	G	F	R	K	M	A	F	P	S	G	K	V	E	G	C	M	V	Q	V	T	C	G	T	T	L	N	G	L	W	L	D	D	V	V	Y	C	P	R	H	
V	I	C	T	S	E	D	M	L	N	P	N	Y	E	D	L	L	I	R	K	S	N	H	N	F	L	V	Q	A	G	N	V	Q	L	R	V	I	G	H	S	M
Q	N	C	V	L	K	L	K	V	D	T	A	N	P	K	T	P	K	Y	K	F	V	R	I	Q	P	G	Q	T	F	S	V	L	A	C	Y	N	G	S	P	S
G	V	Y	Q	C	A	M	R	P	N	F	T	I	K	G	S	F	L	N	G	S	C	G	S	V	G	F	N	I	D	Y	D	C	V	S	F	C	Y	M	H	H
M	E	L	P	T	G	V	H	A	G	T	D	L	E	G	N	E	Y	G	P	V	D	R	Q	T	A	Q	A	A	G	T	D	T	I	T	V	N	V	L	L	
A	W	L	Y	A	A	V	I	N	G	D	R	W	F	L	N	R	F	T	T	L	N	D	F	N	L	V	A	M	K	Y	N	Y	E	P	L	T	Q	D	H	
V	D	I	L	G	P	L	S	A	Q	T	G	I	D	M	C	A	S	L	K	E	L	L	Q	N	G	M	N	G	R	T	I	L	G	S	A	L	L	L		
E	D	E	F	T	P	F	D	V	V	R	Q	C	S	G	V	T	F	Q	S	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	

Fragment analysis of a molecule with indication of activated fragments based on a jupyter notebook in python for post-processing automation.

CT8 QUANTUM CHEMISTRY
AND MOLECULAR MODELLING

Occigen ☁ 680,000 hours
Jean Zay ☁ 780,000 hours



Pascal Raybaud,
SCIENTIFIC ASSISTANT TO THE DIRECTOR
AND RESEARCHER IFPEN
Céline Chizallet,
PROJECT MANAGER AND RESEARCHER IFPEN
Manuel Corral Valero,
RESEARCHER AND SUPERCOMPUTING
CORRESPONDANT IFPEN

Biology, chemistry and materials

Quantum modelling decodes catalysers

IFP Energies Nouvelles (IFPEN), Catalysis, Biocatalysis and Separation Section

Quantum modelling is a relevant and versatile method for exploring the key properties of catalysts used in various processes such as clean fuel production, biomass conversion, photo-electro-catalysis, etc. The calculation of structural, opto-electronic, spectroscopic, thermodynamic and kinetic properties enables the interpretation of experimental measurements and also helps in designing new experiments.

Thanks to the access to Jean Zay and Occigen supercomputers within GENCI (1.5 million hours), IFP Energies Nouvelles produced simulations based on density functional theory and provided innovative results in 2020 with an impact for catalytic materials.

For the description of rare reaction events, the reaction constants of isomerization and cracking of alkenes, catalyzed by zeolites materials, were determined by constrained ab initio molecular dynamics (AIMD) in the Blue Moon ensemble (PhD thesis, IFPEN with Bratislava Comenius Univ.)^[1]. These kinetic constants are used in multi-scale kinetic models and enable the prediction of the performance of catalysts. Current work focuses on the coupling between AIMD and Machine Learning methods to accelerate the choice of

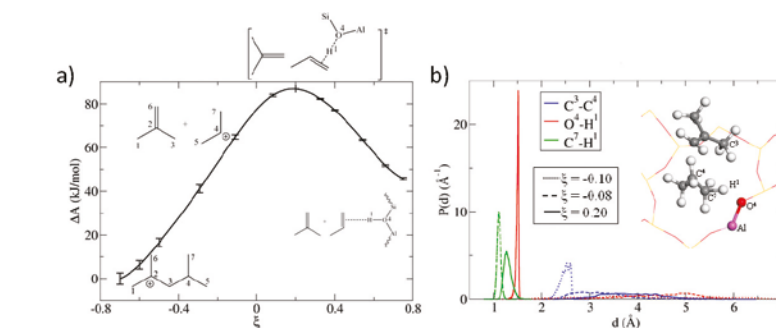


Figure 1. a) Free energy profile computed on the reaction coordinate ξ , by using the Blue Moon ensemble approach for the β -scission reaction of 2-4-dimethyl-2-pentene in isobutene and propene. (b) Probability distributions of distances for various values of the collective variable. The structure shown in the insert is close to the transition state ($\xi=0.2$).^[1]

AIMD collective variables and the shortest reaction pathways (PhD thesis, IFPEN with INRIA).

Thanks to the simulation of complex “nano-rods” models, the structure of metallic particles’ active sites localized on the edges of γ -alumina (γ -Al₂O₃) nano-crystallites was solved and fruitfully compared to NMR spectroscopy and electronic tomography experiments (PhD thesis, IFPEN with CRMN Lyon and IPCM Strasbourg)^[2]. Our research is currently focused on the simulation of the genesis steps of the active phase of catalysts supported on alumina, within the framework of the “Rational Design for Catalysis (ROAD4CAT)” chair (collab. IFPEN with ENS Lyon)^[3].

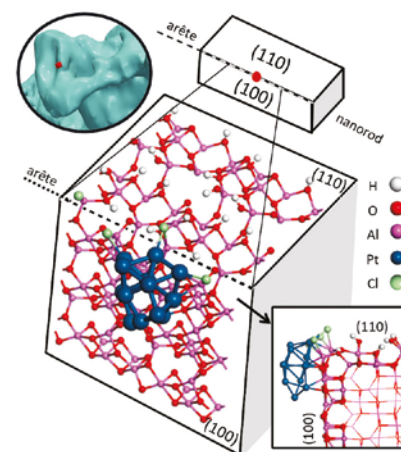


Figure 2. DFT model of a “nano-rod” used for the simulation of a platinum cluster containing 13 atoms located near the edge (intersection of the (100) et (110) facets) of a chlorinated γ -alumina (γ -Al₂O₃) nano-crystallite. The supercell contains more than 500 atoms. The insert represents an electronic tomography image of the real catalyst (platinum cluster in red and alumina in blue).^[2]

[1] J. Rey, C. Bignaud, P. Raybaud, T. Bucko, C. Chizallet. *Angew. Chem., Int. Ed.*, 59, 18938-18942, 2020. <https://doi.org/10.1002/anie.202006065>. J. Rey is co-awardee of the 2020 Y. Chauvin Prize for the best IFPEN thesis. [2] A. T. F. Batista, W. Baaziz, A.-L. Taleb, J. Chaniot, M. Moreaud, C. Legens, A. Aguilar-Tapia, O. Proux, J.-L. Hazemann, F. Diehl, C. Chizallet, A.-S. Gay, O. Ersen and P. Raybaud, *ACS Catalysis*, 10, 4193-4204, 2020. <https://doi.org/10.1021/acscatal.0c00042>. [3] M. Corral Valero, P. Raybaud. *Journal of Catalysis*, 391 (2020) 539-547. <https://doi.org/10.1016/j.jcat.2020.09.006>

**CT7 MOLECULAR MODELLING
APPLIED TO BIOLOGY**

Joliot-Curie ⌚ **6.5 million hours**



Fabio Sterpone,
DIRECTOR
OF RESEARCH
CNRS



Štěpán Timr,
THEORETICAL
BIOCHEMISTRY
LABORATORY, CNRS

Biology, chemistry and materials

The Hamlet curse of a protein: to be or not to be stabilized by the crowd

The function of proteins in our bodies depends on the stability of their native structures, and a loss of this stability may lead to degraded functionality, aggregation, and disease. Proteins generally live in a highly crowded and heterogeneous space, with 5–40% of the cell volume being occupied by different biomolecules. Intuitively, this crowding is

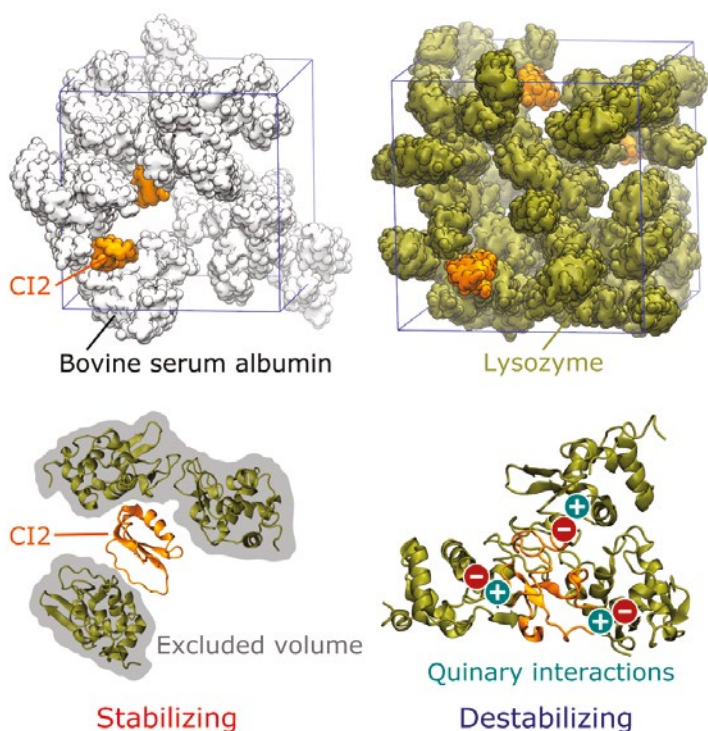
expected to increase the propensity of a protein to remain compact and therefore preserve its native structure. However, the story is a bit more complicated and recent experiments demonstrated that certain proteins can be destabilized by the cell interior. To explain this, one must allow that local interactions between the target protein and its crowded environ-

ment may counterbalance the entropic stabilization. The story is even more complicated since this balance can be modulated by temperature.

It is here where multi-scale simulations come in. We used a combination of coarse-grained simulations based on the Boltzmann molecular dynamics lattice technique with atomistic enhanced-sampling simulations, to examine how different crowded environments impact the stability of a model protein – chymotrypsin inhibitor 2 (CI2).

Our simulations revealed the existence of a crossover temperature above which the crowded environment turns from being destabilizing into a stabilizing one. We were able to identify the origins of this crossover behaviour, namely the increasing importance of the stabilizing excluded-volume effect over the destabilizing attractive interactions with crowders at higher temperatures. Moreover, we found that the total effect depended on the size and other properties of the given crowder molecules. Our results might enhance our understanding of the mechanisms of thermal adaptation in extremophilic organisms.

This work is a part of a long-term computational investigation of crowded biomolecular systems (GENCI 2019/2020 and EU Horizon 2020 project CROWDY) and was recently published in *J. Phys. Chem. Lett.* (doi: 10.1021/acs.jpcllett.0c03626).



(Top) Snapshots from LBMD simulations of the two crowded systems investigated in this work: chymotrypsin inhibitor 2 (CI2) immersed in bovine serum albumin and CI2 immersed in lysozyme. (Bottom) While the native state of CI2 is stabilized by the excluded volume effect, transient weak (quinary) interactions with the protein crowders promote the unfolded state.

CT3 BIOLOGY AND HEALTH

Occigen ⌚ 1.6 million hours



Alain Berod,
DOCTORAL STUDENT
AT SIM&CURE AND IMAG

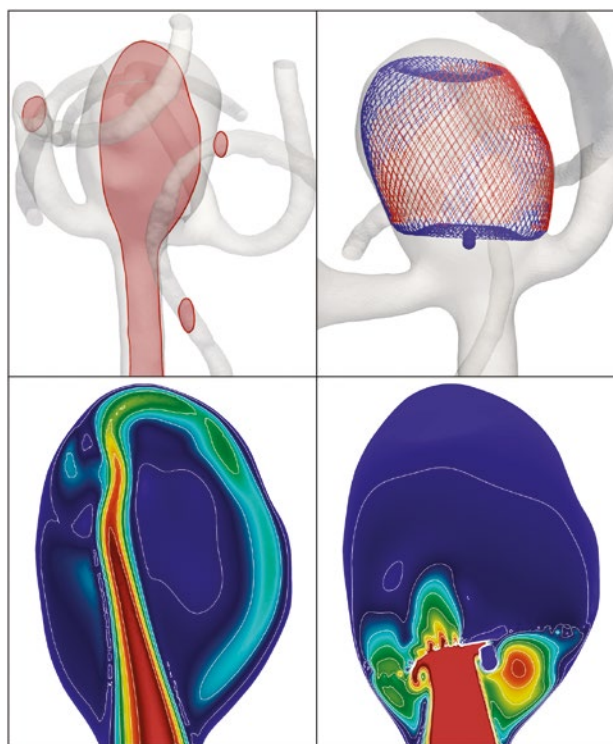
Other applications (computing, health, etc.)

Predicting blood flows in intracranial aneurysms after treatment

Thesis supervised by Franck Nicoud, Simon Mendez and Christophe Chnafa. Sim&Cure is a start-up based in Montpellier (<https://sim-and-cure.com>). IMAG is a joint research unit of CNRS and University of Montpellier (UMR 5149).

Intracranial aneurysms (IA) are local deformations of a few millimeters/centimeters of cerebral arteries harbored by approximately 3% of the general population. The major area of concern about IA is their rupturing due to stresses exerted by the blood on the wall: this rupture may lead to a subarachnoid hemorrhage, with high morbidity and mortality rates. To limit the risk of rupture, dangerous aneurysms have to be treated and over the last few years, endovascular treatments have developed, where a device is implemented locally in the aneurysm or in the parent artery, using a catheter introduced in the patient from the groin or the arm. Such devices are generally made of a number of wires arranged in different ways aiming at preventing high-momentum blood flow in the aneurysm, so that coagulation takes place to stabilize the aneurysm.

In order to predict the success or failure of such treatments, numerical simulation of the blood flow after the insertion of the device is necessary. However, this means resolving the blood flow around the very thin wires, of tens of microns in diameters, of the device. The associated cost would be prohibitive, so that modeling is still required to represent the effect of the endovascular devices on the flow in the aneurysm and further consider to use simulations to predict the medical outcome. The Institute of Montpelli-



*Geometry and flow in an intracranial aneurysm treated with a WEB device (MicroVention).
Bottom: simulations of the flow before and after treatment.*

Top: maps of velocity magnitude from blue (low speed) to red (high speed) at peak systole.

Credits: A. Berod (IMAG, Sim&Cure), C. Chnafa (Sim&Cure), S. Mendez (IMAG) and F. Nicoud (IMAG).

er Alexander Grothendieck (IMAG, CNRS and University of Montpellier) is working with the startup Sim&Cure (<https://sim-and-cure.com>, Montpellier) to develop reduced models for the simulation of the flow in treated aneurysms. In his PhD thesis, Alain Berod developed such a model

and tested it in realistic medical situations, using the in-house software YALES2BIO (<https://imag.umontpellier.fr/~yales2bio>). The figure shows the geometry of the arteries, the position of a WEB (MicroVention) endovascular device and the computed flow before and after treatment. ■

CT6 COMPUTING, ALGORITHMES AND MATHEMATICS

Occigen ⌚ 650,000 hours



Alexandre Denis,
SENIOR RESEARCHER,
TADAAminria BORDEAUX
SUD-OUEST TEAM

Other applications (computing, health, etc.)

Improving the competitiveness of the HPC software stack

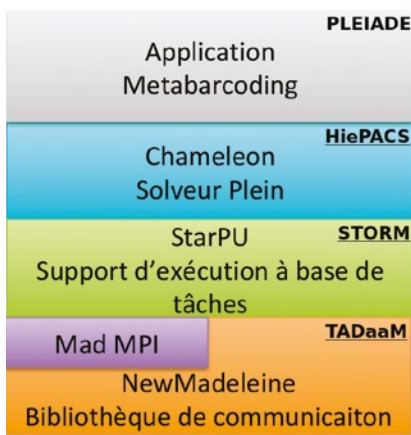
Collaboration between the HiePACS, Storm and Tadaam teams, all 3 from Inria Bordeaux Sud-Ouest

This project involves three Inria teams from the HPC community at Inria Bordeaux Sud-Ouest: HiePACS, Storm and Tadaam. Each of these teams has developed an independent brick for the HPC

software stack: the Chameleon numerical solver, the StarPU runtime system, and the NewMadeleine communication library. These software bricks are each already competitive and recognized by the community. We want to consolidate and improve interfaces between each of them so as to get a better software stack.

of the software stack for better scaling and have been able to solve a very large problem (1 million individuals), at a scale never envisioned before, by using the Occigen computer at Cines.

Figure 1.

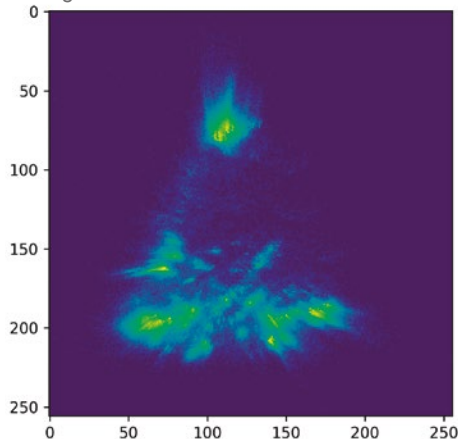


We have worked on the application of individual (micro-organism, eukaryots) classifications, a problem brought to us by our colleagues at the Pleiade team (INRAe partner). With samples ranging from thousands to millions of individuals, robust classification methods relying on SVD (Singular Value Decomposition) are not possible within a reasonable timeframe. A new class of methods, Random SVD, makes it possible to solve the problem on very large scale data sets, by using classical linear algebra algorithms (matrix product, QR decomposition, SVD).

The biggest obstacle we encountered was the handling of the I/O disks, with 750GB of data needing to be loaded before computation. Particular attention needed to be paid to these I/O operations, with the use of StarPU tasks to pipeline reads from disk, data redistribution and the computation itself.

This project enabled us to consolidate the various software bricks, as well as to build synergies between the teams.

Figure 2.



We have integrated the metabarcoding software DIODON, developed jointly by Inria and INRAe, into the software stack. We have worked on each of the bricks

Figure 1. Software stack from the HPC teams at Inria Bordeaux Sud-Ouest.

Figure 2. Heatmap of the projection on the first two axis of a point cloud composed of 1,000,000 sequences (diatoms of Lake Geneva) by MDS. Produced by ADT Gordon on Occigen at Cines.

CT10 NEW APPLICATIONS AND MULTIDISCIPLINARY APPLICATIONS OF HPC

Jean Zay ☉ **150,000 hours**
out of a total of **2 million hours**



Pierre-Yves Oudeyer,
DIRECTOR OF RESEARCH AT THE
INSTITUT FRANÇAIS DE RECHERCHE EN
INFORMATIQUE ET AUTOMATISATION AND
HEAD OF INRIA AND ENSTA-PARISTECH
FLOWERS TEAM

Other applications (computing, health, etc.)

DeepCuriosity: Exploration guided by curiosity and developmental learning in AI

Flowers project team (Inria, Univ. Bordeaux, Ensta ParisTech)

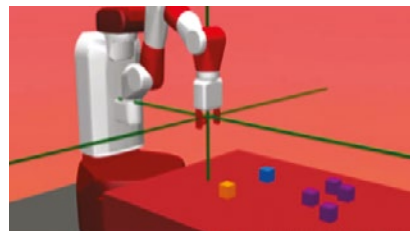
The research vision and program of the DeepCuriosity project is to develop the foundations of a new scientific approach to autonomous artificial intelligence and lifelong machine learning. While deep reinforcement learning has achieved impressive results recently (e.g. in complex board or video games, in robotics, transportation and medicine), it is now reaching both conceptual and practical limits. In particular, current AI systems are far from autonomous: they are still task specific; they require a lot of data and energy; they also require the intervention of engineers for each new task.

To go beyond these limits, the approach proposed in this project is grounded in a decade of interdisciplinary work produced by PY Oudeyer and his team at Inria Bordeaux Sud-Ouest, modeling mechanisms of infant learning and development in humans, in particular curiosity-driven learning. This has set the groundwork for a new machine learning framework: intrinsically motivated goal exploration processes (IMGEPs). In IMGEPs, machines autonomously learn open repertoires of skills by self-supervised acquisition of world models, through sampling their own goals with curiosity-driven self-organized curriculum learning. These algorithms reuse

advances in deep reinforcement learning, integrating them in an architecture which enables autonomous goal generation. Applications on which we work range from video games, robotics, personalization in educational technologies, to tools for autonomous discovery in the sciences.

This work requires experimental campaigns with very large scale computing, in particular to obtain robust results on

the behaviour of these algorithms in various contexts (for this we are looking at a total of 2 million hours of GPU and CPU). For example, one experimental campaign for evaluating one instance of an IMGEP algorithm, with its comparison with other algorithms, involves training neuronal models with several million parameters, and repeating the training and tests in various environments, corresponding to around 200 million hours of GPU. The DeepCuriosity project aims to deploy some ten such experimental campaigns, helping it make progress towards its various stated scientific objectives.



Examples of virtual environments in which intrinsically motivated deep reinforcement learning algorithms are evaluated.

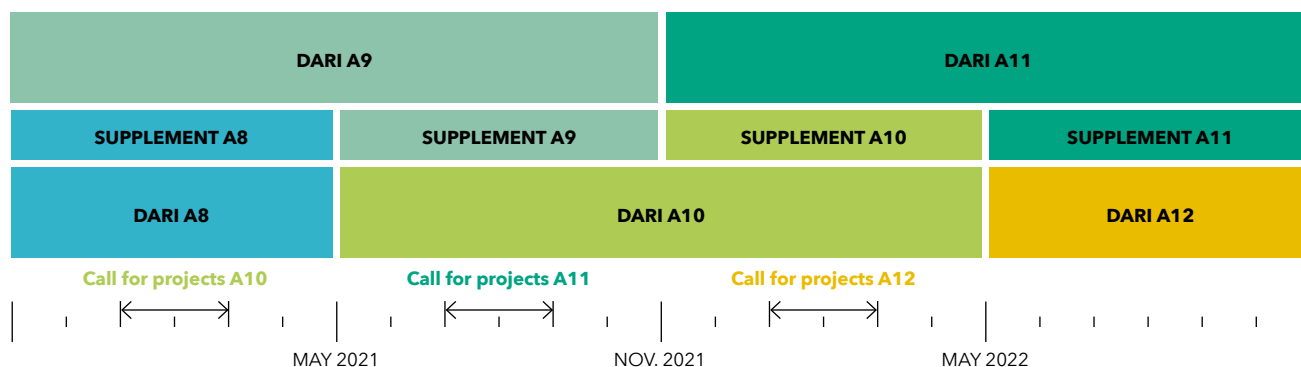
DARI - Resources available for academic and industrial open research

The national computing and storage resources are available free of charge for academic and industrial scientific projects. The project manager must publish the results of work produced using the national resources allocated, in order to stimulate scientific advances and make publicly funded research information freely available. All DARI (Demande d'Attribution de Ressources Informatiques, Computer Resources Allocation Request) applications must be submitted using the www.edari.fr portal, common to all three national computing centers (TGCC, CINES and IDRIS). The various types of access to GENCI's national resources enable it to meet the diverse needs of users. Preparatory Access enables the porting, optimisation and parallelisation of computing codes for migration to the scale of the new architectures. Regular Access is specific to High Performance Computing (HPC) and the use of Artificial Intelligence (AI). Lastly,

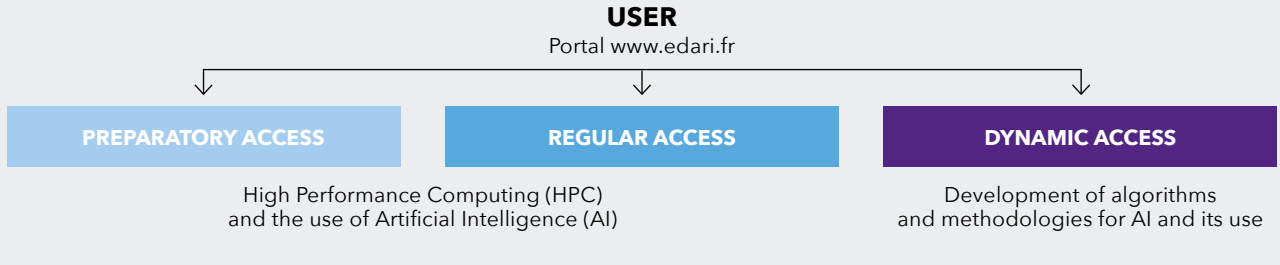
Dynamic Access enables the development of algorithms and methodologies for AI and its use.



Timetable for upcoming DARI allocations



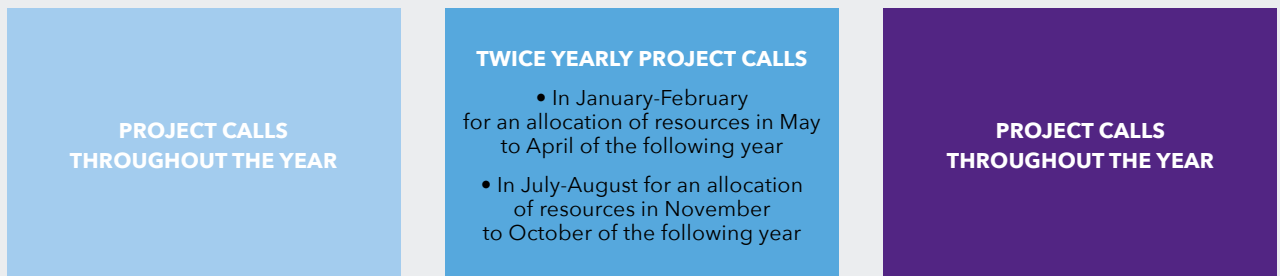
HOW TO APPLY FOR COMPUTING TIME?



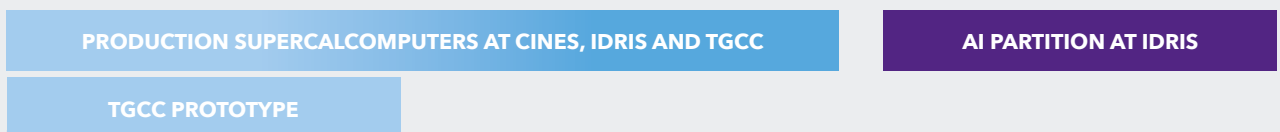
VALIDITY OF RESOURCE ALLOCATION



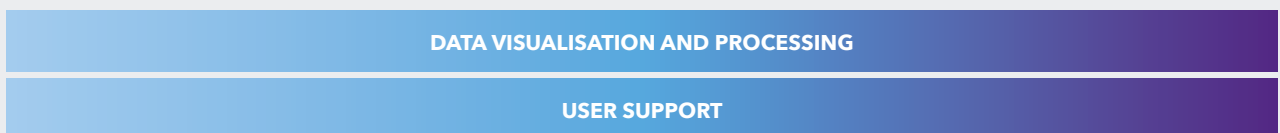
APPLICATION PERIOD



NATIONAL RESOURCES

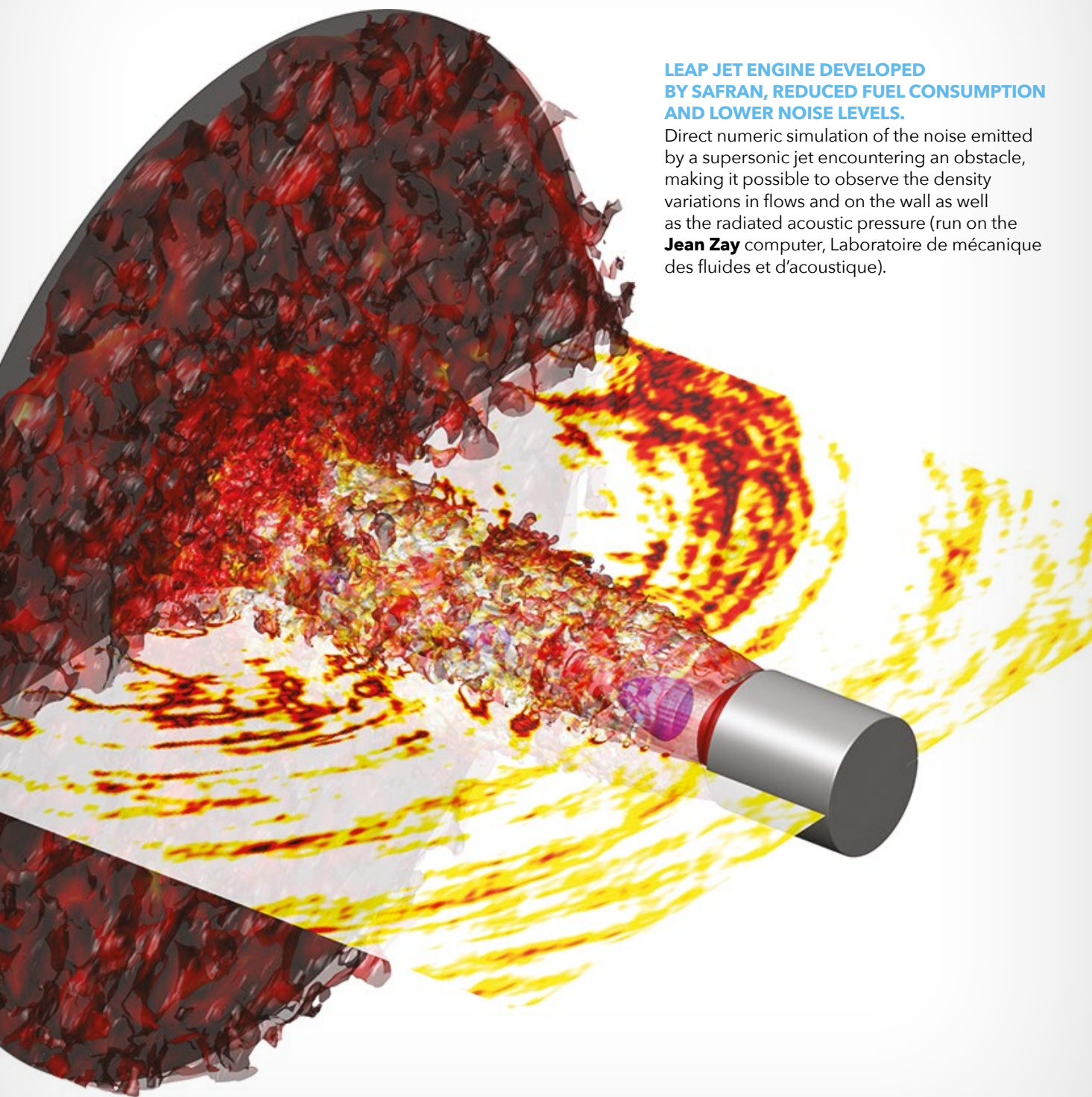


SERVICES AVAILABLE



POSSIBLE ACTIONS





LEAP JET ENGINE DEVELOPED BY SAFRAN, REDUCED FUEL CONSUMPTION AND LOWER NOISE LEVELS.

Direct numeric simulation of the noise emitted by a supersonic jet encountering an obstacle, making it possible to observe the density variations in flows and on the wall as well as the radiated acoustic pressure (run on the **Jean Zay** computer, Laboratoire de mécanique des fluides et d'acoustique).

Industrial results

Collaboration between a research centre, an SME and a Major company for a world first

As an illustration of how industry (SMEs and Major companies) is making use of the computing resources of GENCI in 2020, what better than a world first in the field of aeronautics!

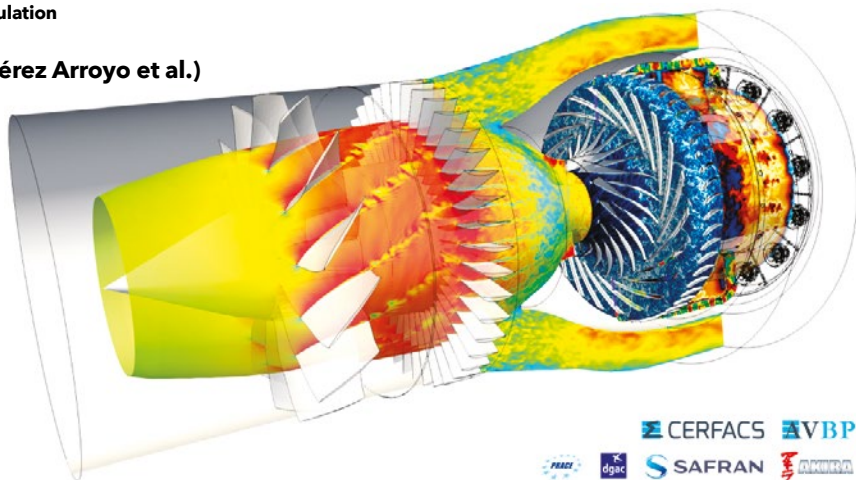
As part of a project entitled FULLEST (First FULL engine computation with Large Eddy SimulaTion) submitted to the PRACE consortium, a team resulting from a collaboration between CERFACS, the SAFRAN group and the SME AKIRA Technologies produced the world's first high fidelity simulation of a complete engine section (from the fan to the combustion chambre). This was a large scale simulation including a total of 2 billion cells, run using the AVBP code from CERFACS. The project was allocated 15.8 million computing hours on the Joliot-Curie SKL partition.

The image shows the various components of an engine and reveals the strong interaction between the high pressure compressor

and its environment, via an upstream impact because of the blower, generating noise, and downstream towards the combustion chambre. This instationary high fidelity simulation of the complete engine was designed as a numerical experiment to validate and improve more low fidelity simulation codes and to study complex physical phenomena, intuited by the experimental researchers and designers but which have not as yet been demonstrated because of the impossibility of instrumenting a real aircraft engine.

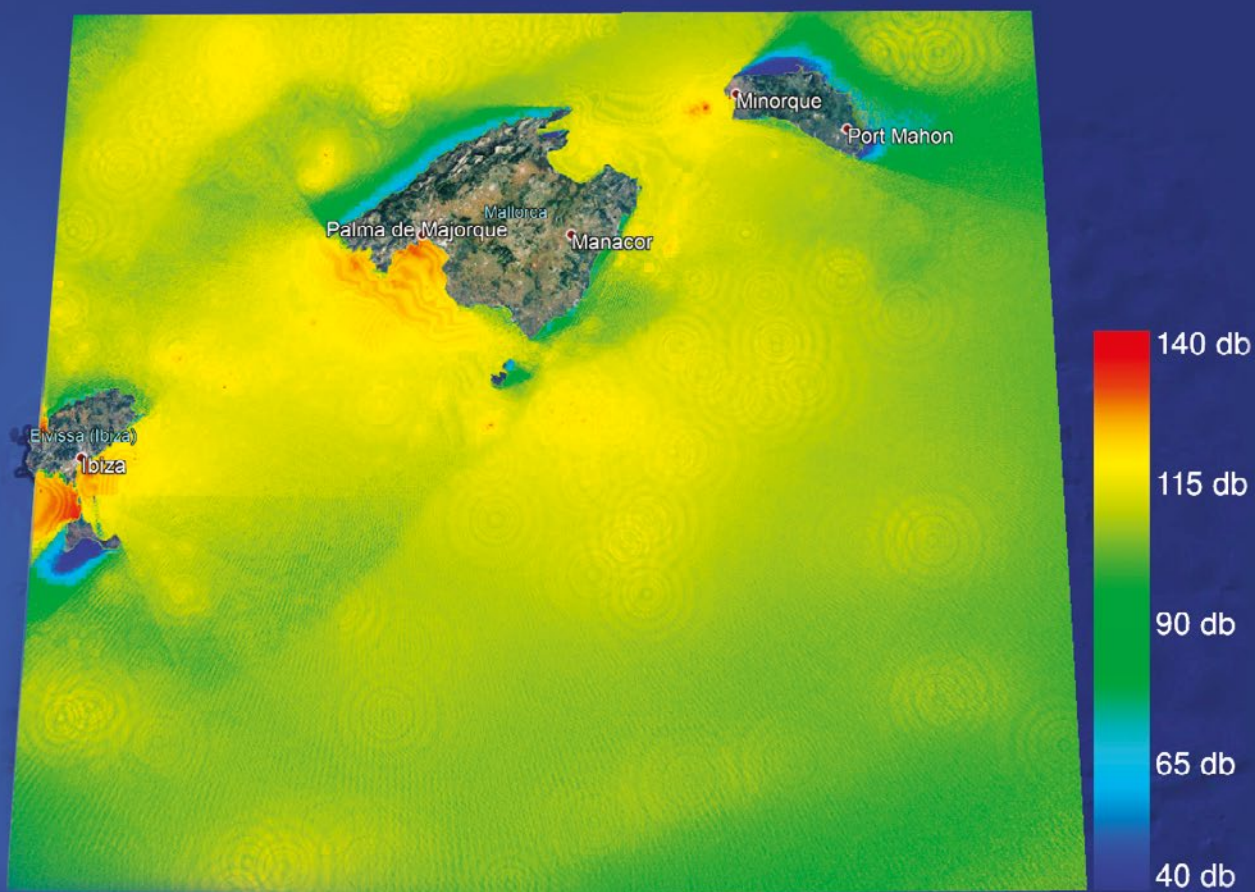
This marks a significant step for the aeronautic industry that will enable the earlier analysis of integration and installation effects and thus reduce the length and cost of the design for future aircraft engines. This project was awarded the Digital Simulation and Artificial intelligence Trophy by Usine Digitale – Teratec!

First full engine computation with large-eddy simulation
PRACE allocation FULLEST - DGEN380
360° simulation with the AVBP code (Pérez Arroyo et al.)
 These results benefitted of funding or developments from projects ATOM (DGAC/SafranTech N° 2018-39), EXCELLERAT (H2020 823691) and EPEEC (H2020 801051)



**ACOUSTIC APPLICATION
DEVELOPED BY SINAY.**

Modelling of submarine noise with a very high level of resolution and covering large areas carried out thanks to the computing power of **CRIANN**.



Startups and SMEs results

GENCI joins the SYSTEMATIC competitiveness cluster

The Systematic Paris-Region competitiveness cluster brings together and runs an excellence ecosystem of 900 members, dedicated to Deep Tech, as well as to major economic and societal issues. The Cluster acts to accelerate digital projects through collaborative innovation, fostering SMEs, networking and sourcing business.

Within the cluster, the Digital Engineering Hub addresses two essential elements: fostering the emergence and development of new design activities required by technological change, and supporting the digital transformation of our environment being driven by new uses. The Hub's ambition is to develop an ecosystem of players capable of jointly meeting the challenge of producing suitable design environments, developing the necessary skills and know-how. These design capabilities obviously require computing infrastructures capable of delivering sufficient power and the storage capacity needed for these activities. Supercomputers, Big Data, modeling, systems engineering and quantum computing are therefore all major challenges placed at the heart of the Digital Engineering Hub.

It is because the activities of the cluster reflect those of GENCI that we joined the Systematic competitiveness cluster in November 2020 and will become part of the Digital Engineering HUB in 2021.



SIMSEO SUPPORTING THE DEVELOPMENT OF THE SINAY SME

Created in 2008, SINAY is helping speed up digitalisation within the maritime sector with the provision of a big data platform and artificial intelligence technologies, machine learning and deep learning.



The SINAY "turnkey" platform - a highly effective web interface - allows maritime operators to view, by means of customised dashboards, their performance indicators and thus optimise their day-to-day operations.

In 2017, SINAY needed to model underwater noises at a very high level resolution and covering a large area (the Mediterranean). The company's in-house systems were not capable of computing on this scale. It was thus decided to work with CRIANN to make use of their computing power.

At the end of 2017, SINAY made its first visit to CRIANN and joined the SIMSEO programme. SINAY's engineers were given a training session and personalised support in implementing the codes on the computer and on how to make best use of the resources.

Performances were accelerated with the development of a parallel version of the code which, coupled with the use of the computer, resulted in a very significant reduction in the computing time to complete the modelling.

Results achieved

- Very significant reduction in computing time: several years down to a matter of hours.
- Modelling capacity covering large geographic areas.
- Accelerated development of the Acoustic application.

Our services for companies, SMEs and Start-ups

SME, Start-up! Get the benefits of large scale computing power for your R&D projects, for designing and developing your concepts and/or products, for developing and identifying new markets or enhancing your competitiveness. The SIMSEO programme supplies you with the expertise of the men and women associated with these computing resources.

You are working in a private R&D laboratory or you are a CEO. You have a research project that needs specialist expertise, numerical simulation, HPC or AI? There are 6 regional computing centers you can access through the SIMSEO programme (www.genci.fr/fr/content/simseo).

Contact SIMSEO and access computing time and dedicated support. You can receive a subsidy of 50% from BPIfrance to help finance your project.

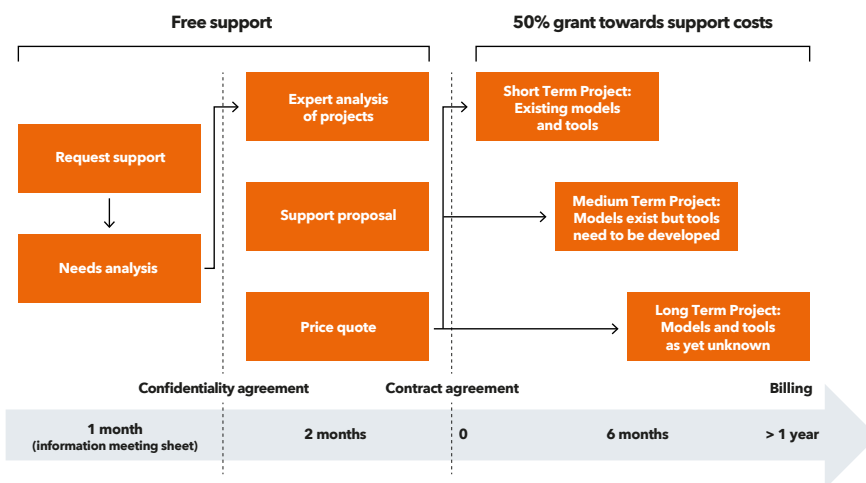
Since the programme started in 2015, 2,128 SMEs have been introduced to the potential and 58 support projects have been completed.

Watch the video about SIMSEO 



Accessing SIMSEO resources

For advice and support



Financing details

Audit of your project

- Checks that your project comes within the SIMSEO programme criteria
 - Does your project involve simulations or AI?
- Is your company registered on the Register of Companies?
 - Is your company French?
- Is your company a start-up, an SME or a mid-sized business?

Submission of a global quote from our teams

Quote drawn up after discussions and analysis of your needs. The 50% SIMSEO subsidy is deducted directly from your price quote. You do not need to make any cash advances. On top of this, the project is also eligible and cumulable with Research tax credits or Innovation tax credits.

Signature of the contract

Confidentiality agreement, if needed.

Billing for SIMSEO service provisions

- There are 3 modes, and depending on the platforms:
 - After the end of the project.
- With intermediate payment depending on the projects.
- As a pay-as-you-go mode for computing hours used.

SIMSEO, TRADE SHOWS AND WORKSHOPS



AI WORKSHOP: USING SUPERCOMPUTERS TO BOOST YOUR PROJECTS WITH GENCI - 25 JANUARY 2020 AT THE FRENCH TECH CENTRAL AT STATION F.

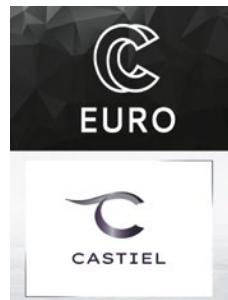


BIG DATA AI PARIS 2020 FAIR - PORTE DE VERSAILLES ON SEPTEMBER 13, 2020: SIMSEO PROGRAM PRESENTATION WORKSHOP, INCLUDING THE SINAY START-UP.

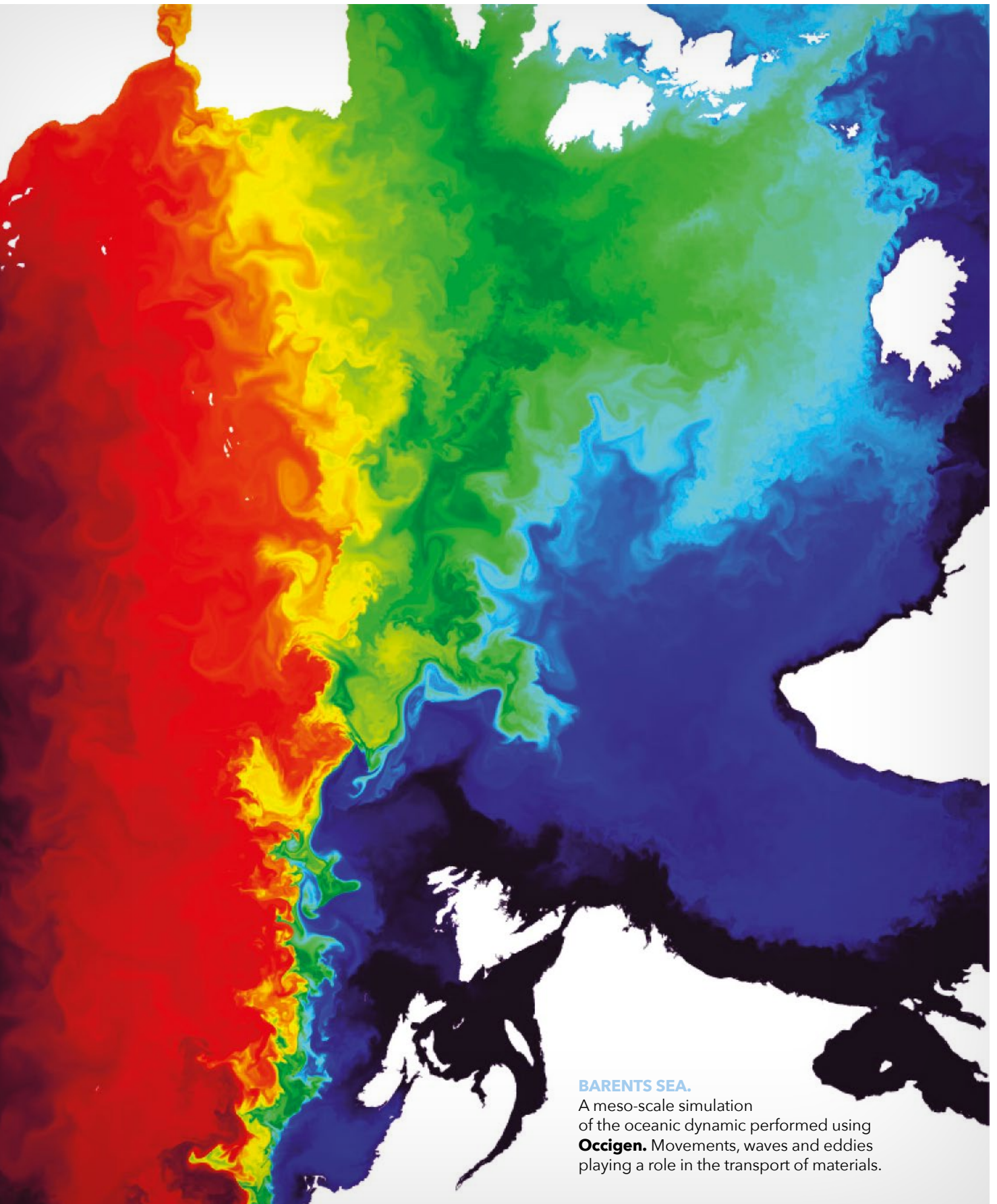
Competence Centers (CASTIEL & EuroCC projects)

As part of the EuroCC Horizon 2020 (H2020) project of the European Union, each of the 33 participating countries is tasked with creating a unique National Competence Center (NCC) for High Performance Computing (HPC), High Performance Data Analysis (HPDA) and Artificial Intelligence (AI).

These NCCs will coordinate activities in all areas related to HPC and serve as a point of contact for customers from industry, science, HPC experts and the general public. The EuroCC project is funded 50% through the EuroHPC Joint Undertaking (JU) and 50% through national funding programs. The overall objective of EuroCC is to create a European base of excellence in HPC by filling existing skills gaps and offering a broad portfolio of services in the areas of HPC, HPDA and AI, tailored to the needs of industry, academia and public administration.



EuroCC works in close collaboration with the CASTIEL (Coordination and Support for National Competence Centers on a European Level) Coordination and Support Action, which links NCCs across Europe in order to contribute to the success of the EuroCC project. CASTIEL promotes collaboration, the exchange of knowledge and skills. ■



BARENTS SEA.

A meso-scale simulation of the oceanic dynamic performed using **Occigen**. Movements, waves and eddies playing a role in the transport of materials.

GENCI today

47 Roll-out of Dynamic Access

48 Technology and innovation

50 GENCI in the regions

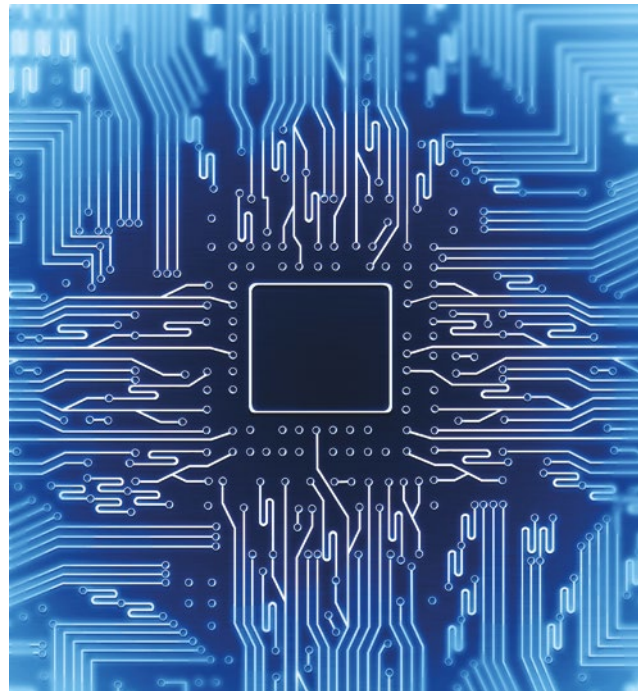
52 GENCI in Europe

Roll-out of Dynamic Access

Initially reserved for Artificial Intelligence on Jean Zay, the examination of possible changes to access modes carried out in 2020, will be given real shape with the introduction of Dynamic Access (DA) in 2021 for all disciplines and all GENCI computers. Following the very positive results for the use of DA for Artificial Intelligence and the desire to have access modes that are comparable and consistent with future access modes for PRACE/EuroHPC, GENCI approved the roll-out of Dynamic Access for all the Thematic Committees in the HPC world and its computers.

This fast and flexible access mode has already enabled more than 400 AI projects to obtain computing resources independently of the biannual Regular Access (RA) allocations since the opening of the computer in October 2019. Eventually, it will be possible for all requests for allocations of less than 500,000 CPU core hours or 50,000 GPU hours to be approved in a matter of days, making it easier for 50% of researchers by providing a more flexible way for them to submit requests for resources.

DA for everyone in 2021!



Technology and innovation

2020 OR THE YEAR OF THE SUCCESSFUL CONVERGENCE OF HPC AND AI ON JEAN ZAY!

With its inauguration in January 2020, the doubling of its computing capacities last summer and the rapid uptake of the Dynamic Access regime (370 projects and 6 million hours allocated), 2020 provided the proof that Jean Zay, the first converged and hybrid computer in France, was critical in boosting Research and Innovation.



communities prepare most effectively for the arrival, in 2023/2024, of Exascale class computers which will also be greatly accelerated and converged, comprehensively combining numerical simulation and the use of artificial intelligence.

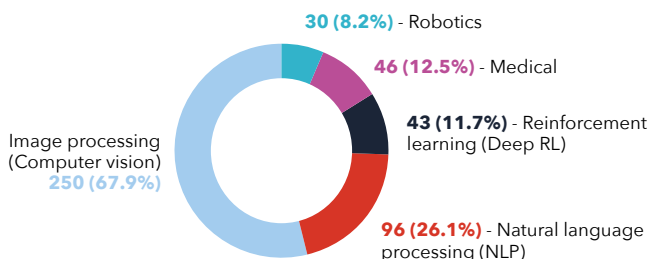
(1) <https://arxiv.org/abs/1912.05372>
 (2) <https://www.gustaveroussy.fr/fr/lintelligence-artificielle-guide-une-prise-en-charge-plus-anticipee-et-personnalisee-de-la-covid-19>

Converged because, thanks to its physical characteristics (including 2,696 nVIDIA V100 16/32GB computing accelerators and a first DDN full flash high speed 2.2 PB to 0.5 TB/s storage space) and software (work scheduler, optimised frameworks, secured container support and Jupyter notebooks, etc.), it is possible to address both needs for numerical simulation (HPC) and Artificial Intelligence (AI), making Jean Zay one of the first systems of this type in Europe.

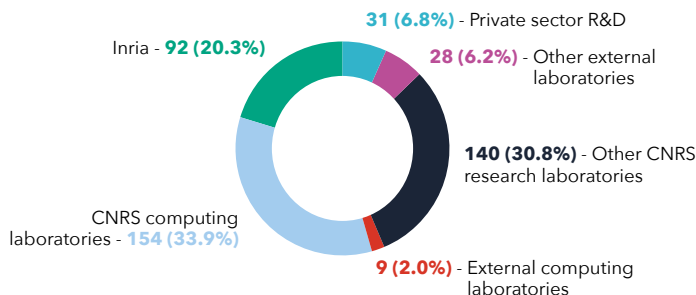
Beyond its initial mission in response to the national *AIForHumanity* plan to deliver sovereign computing power for French Research in AI, Jean Zay has also helped bring together the numeric simulation and AI communities. Thus, whether it is in the post-processing of instrumental and computational data, the increasingly effective coupling between modelling and AI, or the scale out of AI models on several tens of hundreds of GPUs (examples of language processing for the flauBERT project⁽¹⁾ or image recognition with the COVID19 ScanCovIA project⁽²⁾), the scope of use of Jean Zay for academic and industrial research (start-ups, SME, large companies) is constantly expanding.

Jean Zay, together with Joliot-Curie and the upcoming successor to Occigen, are thus complementary computers which, thanks to application support experts, are helping their user

Scientific fields of users for AI on Jean Zay



Laboratories supporting the submission of projects for Jean Zay



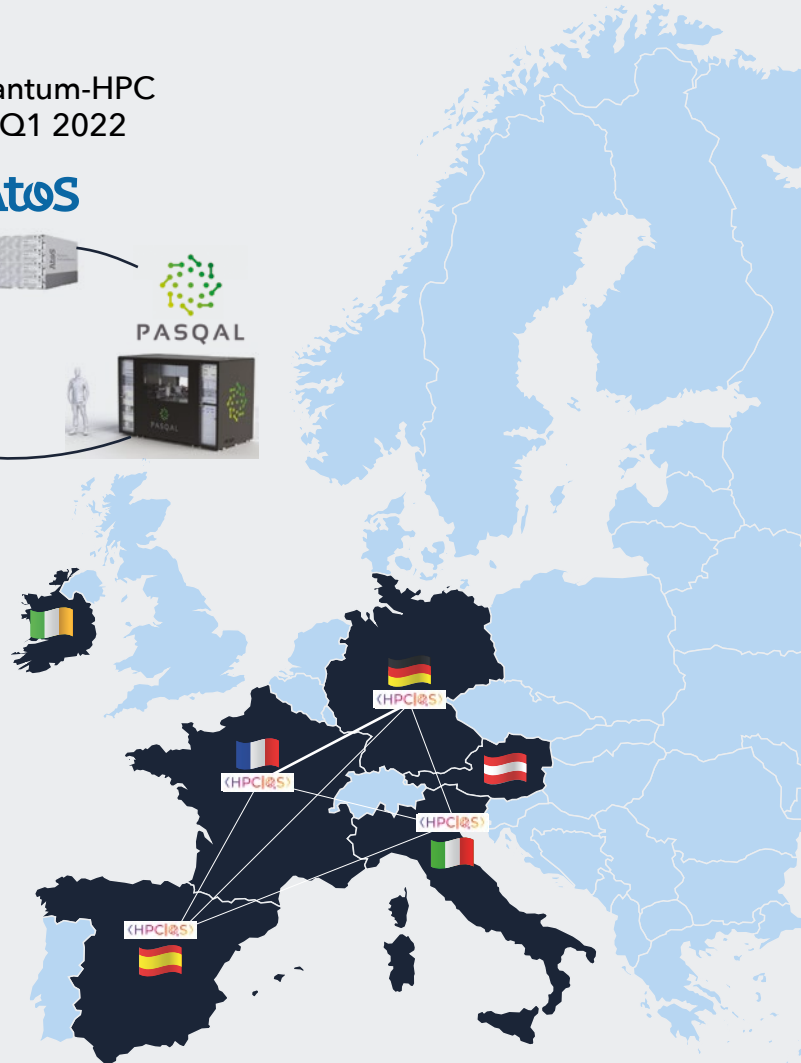
<HPC|Q|S>

The First Cloud-based and hybrid Quantum-HPC European Infrastructure 2x100 qubits Q1 2022



PAck Quantique (PAQ)

Support Industries to assess quantum computing on real use cases thanks to french academic consortia and Quantum startups



TOWARDS QUANTUM

GENCI is contributing, in the context of a EuroHPC (HPCQS) project and the French National Quantum Plan, to the creation of a European quantum hub in cloud mode by installing a hybrid HPC / quantum infrastructure at CEA-TGCC (France), similar to the one to be installed at FZJ-JSC (Germany). The HPCQS consortium is made up 16 European partners including CIN-ECA and BSC, who will each host a EuroHPC pre-exascale class supercomputer in 2021, the Irish national center ICHEC, and 6 French partners including CEA, CNRS, Inria and GENCI as well as 2 French companies, Atos and Pasqal. At the end of 2022, the two Joliot-Curie (TGCC) and Juwels (JSC) supercomputers will each be coupled to a Pasqal Fresnel simulator of at least 100 qubits based on cold atoms excited by laser beams, which is a

world first! These coupled systems will be used through the Atos QLM which has an agnostic programming interface enabling both the consolidation of developments by French and European academic and industrial researchers, and interfacing with future emerging technologies (trapped ions, carbon nanotubes, corrected qubits, quantum photonics, etc.). The HPCQS infrastructure will be one of the pillars for Quantum PAck (PAQ), a €1.5M program funded by the Ile de France region to support industry in its use of quantum computing and with actual demonstrations of its benefits, starting with 3 projects selected in 2020 in the energy (TOTAL, EDF) and bio-pharma (Qubit Pharmaceuticals) sectors. The program will continue in 2021 and could be extended to other regions.

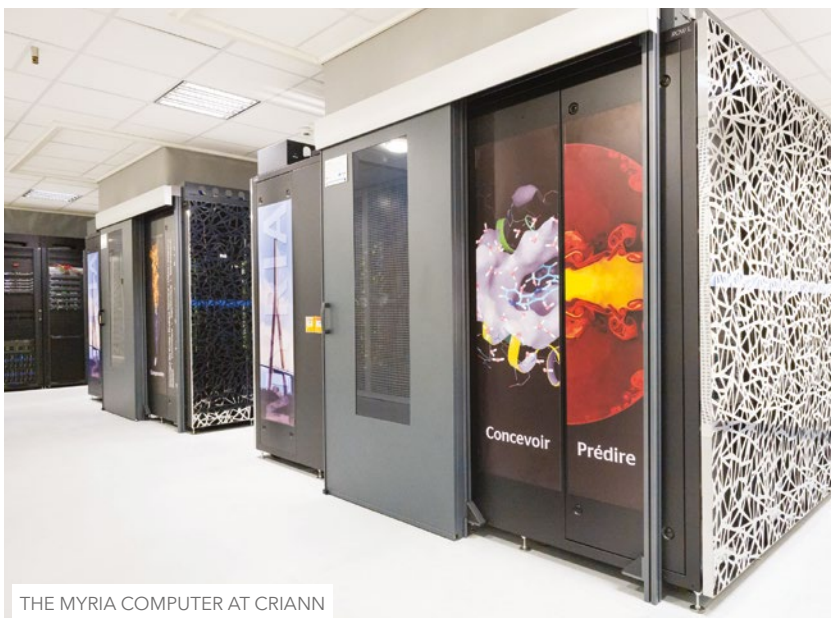
GENCI in the regions

MESONET PROJECT

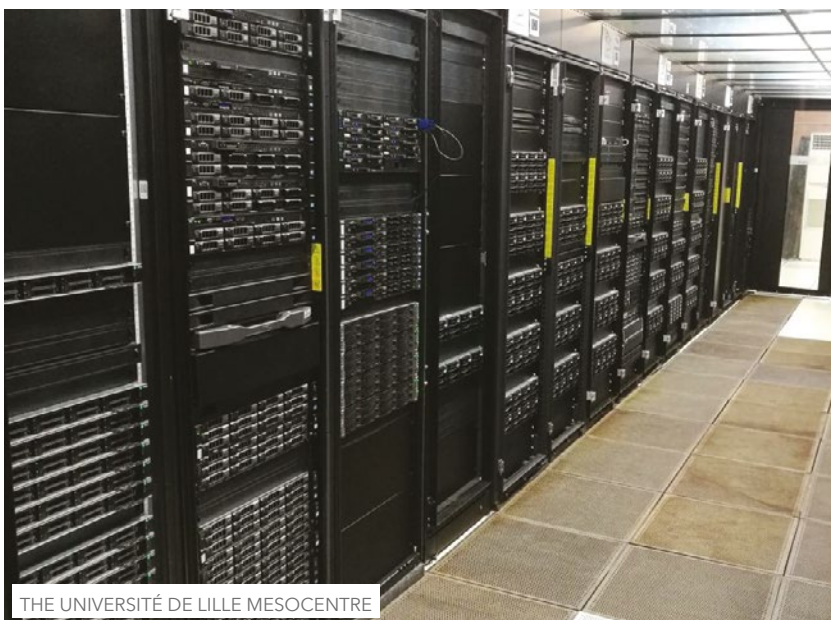
During 2020, and in conjunction with the 21 regional computing centers, GENCI developed the MesoNET project proposal. The long-term objective is to set up a distributed infrastructure dedicated to coordinating HPC-AI in France. It will bring together the qualifying Mesocenters and make them regional references and relays, offering shared access to skills and equipment in the fields of High Performance Computing, AI and data.

The resulting national and regional infrastructure should then significantly increase the understanding and use by researchers of national and regional public digital infrastructures, in particular for emerging research communities (human and social sciences, etc.). As these resources are fully integrated into national and European programs, they will also be available within the framework of the European Open Science Cloud initiative (EOSC).

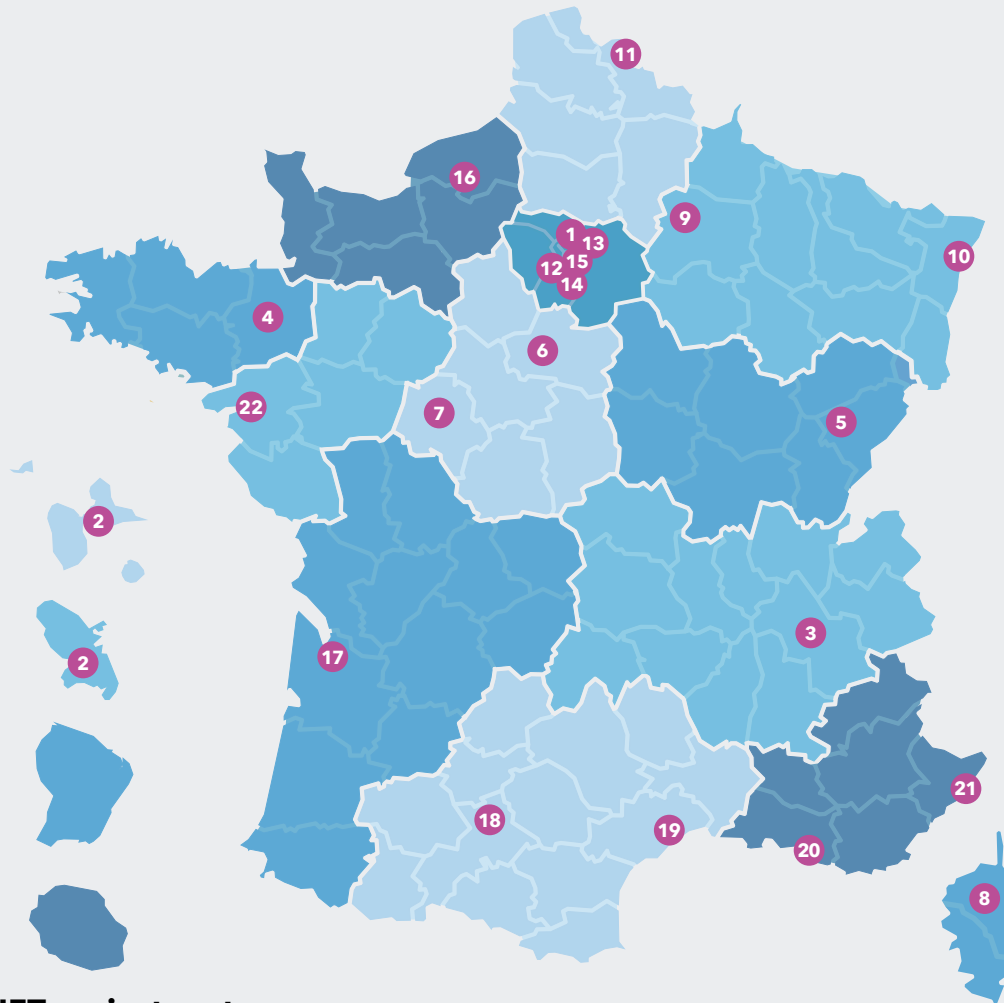
This project was accepted as part of the ESR/EquipEX+ on December 18, 2020, and covers a 6-year period (2021-2027).
























THE MYRIA COMPUTER AT CRIANN



THE UNIVERSITÉ DE LILLE MESOCENTRE



MesoNET project partners

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

GENCI in Europe



PPI4HPC PROJECT "WHITE PAPER"

In the context of the PPI4HPC project, financed by the European Commission, a group of buyers (BSC for Spain, CINECA for Italy, JSC for Germany and GENCI/CEA for France) was established to execute a joint public procurement of innovation solutions (PPI) for the first time in the field of High Performance Computing (HPC). This project is seen as being a test bench in evaluating the usefulness of PPI for the bigger future joint pan-European operations that will be launched under the EuroHPC initiative.

The partners worked together on the coordinated roadmaps and on the awarding of a joint contract, for which GENCI will be responsible, for the supply of optimised computing and storage resources in response to European scientific requirements.

At the end of this procedure, a "White Paper" was drawn up to explain, with an emphasis on the legal elements acquired, how the public sector buyers involved in the project had prepared and successfully completed a joint procurement of innovative equipment. It identified a series of recommendations, based on lessons learned, that should be of value for future joint European public procurements:

- The formation of motivated and primed teams as of the initial stages of a project is key to its success.

- Legal advice is very important and it recommended involving a legal firm specialising in the relevant legal aspects, not just in the country of the leading buyer but also in the countries of the local buyers.
- A clear definition of the roles and responsibilities of the various partners during the entire contract awarding procedure (formalised in a joint contract awarding agreement) is necessary to ensure harmonious relationships between the partners throughout the process.
- Extensive and fair information on the contract must be made available.
- The awareness of all players involved on the sites awarding the contracts of the legal procedures and the exchanging of information throughout the execution of the local contract awarding procedures was identified as an important aspect.

Finally, for the technical aspects and relating to the French lot, it is worth noting that PPI4HPC enabled the extension to the capacities of the Joliot-Curie computer at TGCC with a manycore partition (12.67 Pflop/s with AMD Rome processors), an accelerated partition (with nVIDIA V100 GPUs) and in mid-2021 a partition equipped with Arm Fujitsu A64FX processors. ■





◀ SIGNATURE OF A COLLABORATION AGREEMENT BETWEEN PRACE, CERN, SKAO AND GÉANT IN JULY 2020.

INTENSIVE ACTIVITY ON THE EUROPEAN STAGE!

Despite the health crisis that has seriously slowed work on European projects, 2020 was the year that saw the transition towards the new missions of EuroHPC and new uses of HPC in Europe.

Thus as part of the PRACE-6IP project which supports the operational activities of the PRACE infrastructure, a collaboration agreement was signed between PRACE, CERN, SKAO (the organisation managing the SKA world radiotelescope project) and GÉANT (the European research project) in July 2020. This covers, with the creation of demonstrators, the challenges of the end-to-end management of big data (soon to be several hundred Pb of raw data a year) by workflows through fast networks from the instrument (edge) to the computer centre (HPC/Cloud) using methods combining HPC and Artificial Intelligence (AI).

With the deployment of the EuroHPC initiative and the ongoing discussions between PRACE and EuroHPC for the supply of value added HPC services, the PRACE-6IP project has been partly re-focused to strengthen activities around the allocation of resources (peer review), training, applications and technology watch (in liaison with the INFRAG and RIAG committees of EuroHPC) and communication (conference organisation). These changes were welcomed by the European Commission during its (positive) evaluation of the project in December 2020.

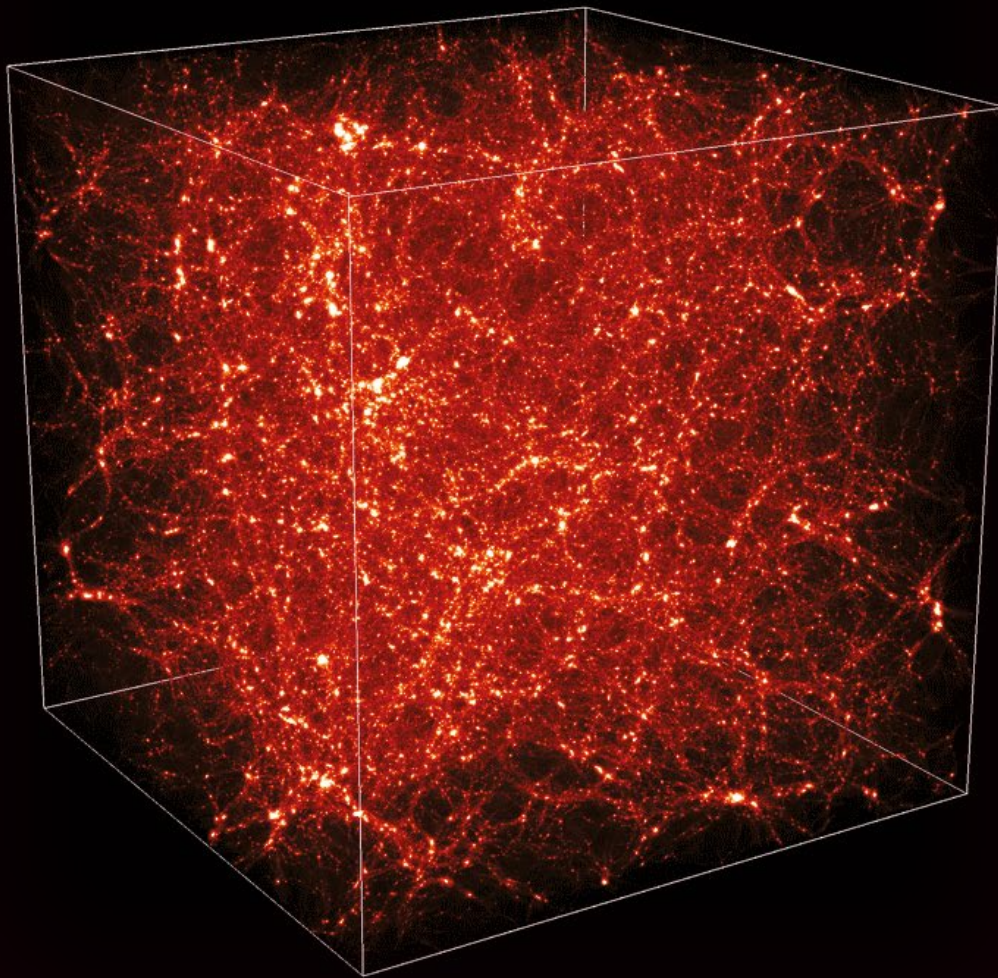
Again in the field of new uses, the AQMO project came to an end on 31 December 2020. Its objective was to deliver, for the Rennes metropolitan area, an integrated end-to-end data management platform, from the sensors located on the local Keolys buses to the Jean Zay supercomputer at IDRIS, for air quality simulations/forecasting, thereby improving current practices in terms of measurements. An end of project seminar was organised to disseminate the results through a two-hour film (<https://www.youtube.com/watch?v=YCbprc58YJ>). The next stage will be the operational deployment of this type of service in one or more smart cities, which will carry the use into the future.

Finally, because of the COVID-19 pandemic, PRACE offered fast track access to its supercomputers for those researching in this area. A total of 35 projects were able to access the resources of PRACE including Joliot-Curie at TGCC. On top of this, the Commission launched a series of project calls in support of research efforts. CINES, representing TGIR GENCI, was involved in one of the selected project (dubbed ORCHESTRA) focusing on the sharing of data from COVID-19 cohorts. This project, which included INSERM on the French side, consisted of a section dedicated to the processing of data prior to their centralisation on a platform hosted in Italy (University of Bologne, project manager). ■

**INITIAL HETEROGENEITIES
IN THE UNIVERSE.**

A numeric simulation carried out on **Joliot-Curie** at CEA on the formation of the structures of the Universe.

The image uses false colours to show the 3D distribution of mass in a one billion light-year cube. The simulation involved almost one billion particles and meshes.



GENCI tomorrow

Towards Exascale and beyond



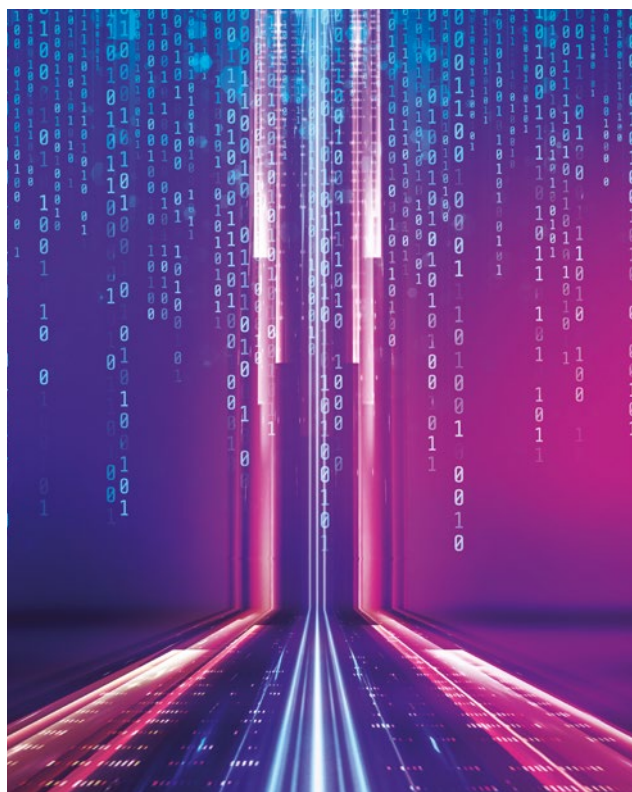
In the context of the rollout of its activities, the European EuroHPC initiative (currently consisting of the European Commission and 33 Member States) has just announced the creation of a pan-European computing infrastructure bringing together, gradually as of March 2021, 5 multi Petascale class systems (in Luxembourg, Portugal, Czech Republic, Slovenia and Bulgaria) and 3 pre-Exascale class systems (with a peak power of 400 to 550 PFlops, hosted in Finland, Italy and Spain).

With these systems coming online shortly, it is now focusing on the next stage in the deployment, Exascale, these are systems that are at least twice as powerful and comparable to those that will be entering service in the United States, China and Japan between 2021 and 2023.

The Minister of Higher Education, Research and Innovation has announced the intention for France to bid, through GENCI, to host, at CEA TGCC, one of the two EuroHPC Exascale computers planned as of 2023/2024.

For this purpose, GENCI and its associates have developed an integrated project to bring together all the technical, scientific and financial elements to enable it to submit its proposal in the next EuroHPC project call which is expected at the end of 2021. It covers in particular:

- the creation, as was the case with the pre-Exascale computers, of a consortium of national (academic and industrial) and international partners for the joint funding of the 50% of the full cost of these systems over 6 years;
- a proposal for the joint undertaking (JU) the details of the architecture (computing, storage, computing environment) for a converged Exascale machine (HPC, AI and HPDA), using scalar resources (possibly using a processor resulting from the European EPI - European Processor Initiative – project),



- but above all accelerated resources (mainly based on accelerators) but possibly including, depending on the outcomes of the HPCQS project, for certain target applications, quantum accelerators, and not forgetting the big data processing element;
- and finally, a survey and an estimate of the needs of the user scientific communities in terms of development, support and training.

Women and men working to support research

CHANGES TO THE WORKFORCE

As at 31 December, the GENCI team was 16 strong after the following changes:

- the secondment by CNRS of a Project Manager Engineer as of June 2020,
- the recruitment in September 2020 of a fixed term employee for the Competence Centre project.

This amounted to 13.67 FTE taking into account:

- the ongoing recruitments during the year (prorata temporis over the year),
- the long-term illness of one employee,
- the maternity leave for two employees.

Recruitment is ongoing for the two vacancies (Communication Manager and Project Administration Manager), as well as the position as Exascale Projects Manager as a fixed term contract as of the end of the year.

STRUCTURE OF THE CIVIL SOCIETY DURING THE COVID-19 PERIOD AND GDPR

Governance of GENCI

In accordance with Order 2020-321 of 25/03/20 applicable to meetings held as of 12/03/2020, the Council of GENCI was legally able to meet using audio-visual conferences when it was possible to verify the identity of the members of the meeting present. The members and other persons with a right to attend Council meetings were invited by any effective means informing them of the date and time of the meeting.

The arrangements under the Order apply to all resolutions submitted to a vote by the Council and thus regularly voted on and enabled the legal continuity of the company.

Impact of GDPR on the activities of GENCI

An analysis was initiated at the end of the year on the subcontractor relationship of GENCI and the centers relative to the users of the supercomputers and to the personal Data Controllers (sensitive or not) in the context of projects taking into account health data at Idris. The analysis was performed and allowed GENCI in this specific case to:

- confirm its standing as first level subcontractor;
- identify the actions to ensure compliance in its relations with the centers which are in effect second level subcontractors;
- draw up an action plan to ensure its compliance.

A number of discussion meetings were held with CNRS, then with CNRS DPD which resulted in:

- a convergence on the point of view of the status of GENCI as first level subcontractor;
- an approval in principle for the action plan;
- and a request from CNRS that GENCI implement the suggested actions so that they could be approved during 2021 by CNRS and make it possible to establish a procedure for processing requests relating to health data.

DEPLOYMENT OF THE CLEEMY, FIGGO TOOLS AND EVOLUTION AND CLOSING OF ACCOUNTS AT GENCI

GENCI introduced two tools from Lucca in the 1st quarter 2020 for use by its employees:

- the FIGGO tool is used for inputting leave days, RWD, time off in lieu, sick leave or others, and to view a full breakdown of current entitlement. These absences are then integrated into the employee's diary once validated by the line manager. It also allows the calculation of the number of "tickets-restaurant" (luncheon vouchers) to issue.
- The CLEEMY tool is used for entering costs relating to a mission by dematerialising the expense proofs archived as accounting documents. The line manager is responsible for approving the expense claims of staff members.

EMPLOYEE RELATIONS

Elections of representatives to the Comité Social Economique (CSE) were held at the end of 2019 and a staff representative was elected, enabling the CSE to meet for the first time at GENCI.

The CSE consists of the CEO, the General Secretary and the staff representative. The meetings are held monthly and the first meeting was held on 28 January 2020. The following subjects were on the agenda and approved by the CSE:

- Arrangements for time off in lieu for work related travel if normal working hours are exceeded;
- The drawing up of an IT Charter setting the structural framework;
- Approval of a single work-related risks document (*Document Unique d'Evaluation des Risques Professionnels (DUERP)*);
- An appraisal of remote working experiences. When remote working was implemented in 2019, it was stated that there would be a report on it at the end of a period of one year. The staff were consulted by means of a questionnaire. The responses to the questionnaires were covered in a feedback meeting with staff on 24 November 2020. This has provided the basis for the review by the CSE of modifications to the remote working charter applicable at GENCI.

INTERNAL ORGANIZATION IN 2020

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

Technical and Operations Department



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



Delphine THEODOROU
Project Operations
Manager



Pascal VOURY
Project Operations
Manager



Abraham LUNDA
Technical- Commercial
Projects Manager:
Competence Centre

Communication



Annabel TRUONG
Communication Officer

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

Committees members and Official Bodies

As at 31/12/2020

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 Stéphanie Lê Van.
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*. **CPU 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 Olivier BERARD, *Managing Director for purchases & innovation - Mrs Gwendoline JOLY-JAGOT, 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:** Mr Christophe CALVIN, *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*. **CPU representative:** Mr François 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 Frédéric Desprez, *Deputy Scientific Director for "Networks, Systems & Services"*.

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*. **CPU representative:** Mr Olivier Simonin, *Chairman of National Polytechnique Institute* - Mr Jacques Bittoun, *former Chairman of Paris-Sud University*. **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 2020.

Guaranteeing ever-more powerful supercomputers, making it possible to simulate increasingly realistic models, and processing and analysing the growing mass of data, is a strategic challenge.

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.

On reading this report you will be able to see to just what extent high performance computing is now central to how we live.

High performance computing has impacts for every scientific field, as well as for industry, the SME and start-up sectors, as an accelerator of innovation, as a decision aid and helping find solutions during major crises affecting health and society as a whole, such as the COVID-19 pandemic.

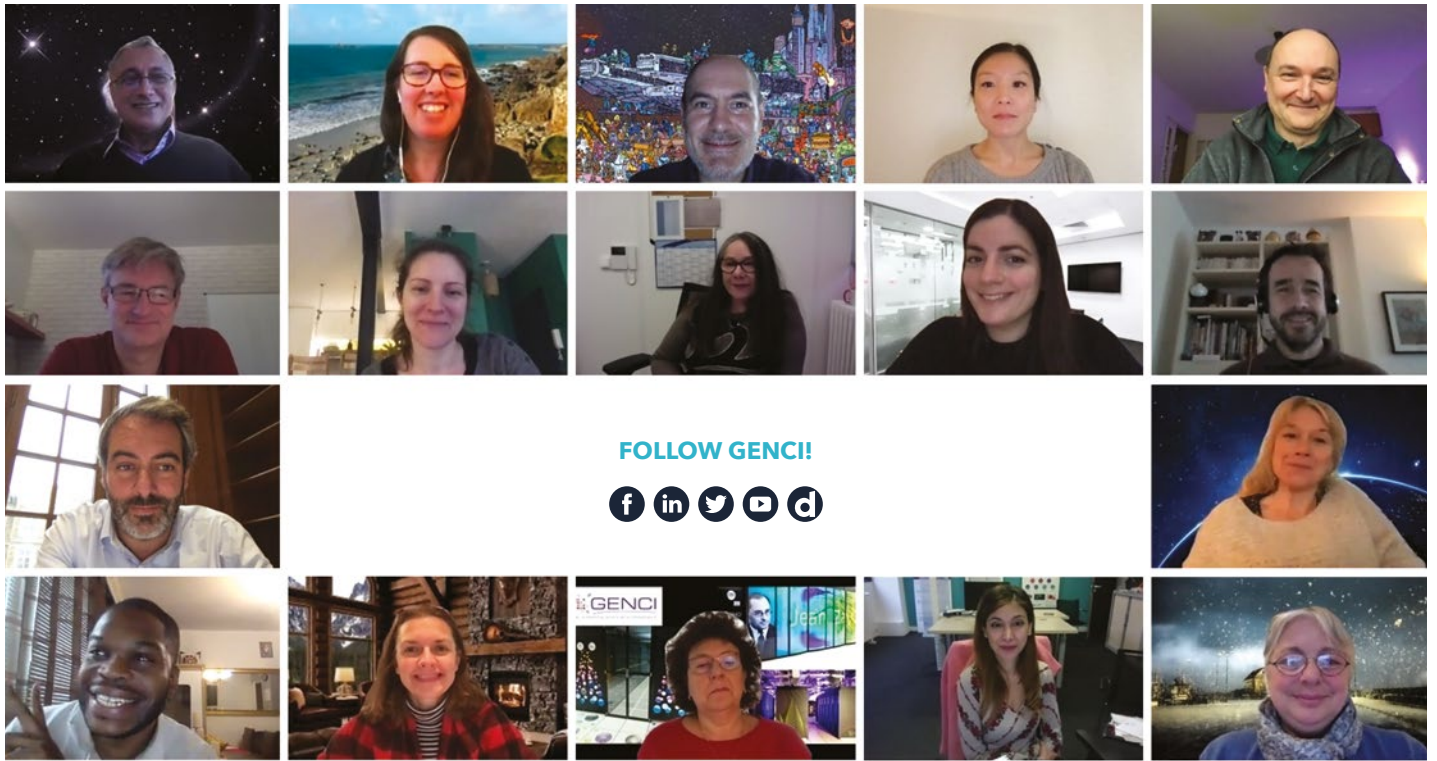
Once again, thank-you so much.



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