ANNUAL REPORT
2019

HPC at the service of knowledge
With the mission to make available high-performance computing and data storage resources, GENCI ensures, at both the national and the European levels, the widest possible use of high-performance computing together with Artificial Intelligence in supporting the work of academic and industrial research teams.
04  **GENCI: at the heart of the biggest challenges**

04._ Foreword from the DGRI
05._ Editorial by the CEO of GENCI
06._ 2019 as seen by GENCI’s shareholders
08._ HPC and Artificial Intelligence, a critical convergence
09._ GENCI’s strategic plan

10  **TGIR Large-Scale Research Infrastructure**

11._ Urbanization, harmonization of services
12._ Technology Watch: evolving prototypes
13._ New opportunities for users
14._ Computing Centers and Supercomputers
18._ GENCI events in 2019
20._ GENCI in Europe and France
22._ Events and Prizes

24  **Impact of GENCI for the scientific community**

25._ Foreword by the Chair of GENCI’s Evaluation Committee
26._ Thematic Committees, forewords by the Chairs
28._ 2019 Main scientific results

40  **Impact of GENCI for start-ups, SMEs and industry**

40._ Our actions in support of start-ups and SMEs
41._ Our actions in support of industrial competitiveness

42  **GENCI, at the service...**

43._ ... of research and innovation
43._ ... of users

44  **GENCI: Internal Organization**

45._ Latest on the Civil Society
46._ Internal organization
47._ Members of the Official Bodies

Follow GENCI at [www.genci.fr](http://www.genci.fr), on our Youtube channel (GENCIVIDEOS) and on Dailymotion (tv-genci), as well as through the social networks:
2019 was a momentous year for GENCI, with a large workload in terms of the renewal of equipment at TGCC and IDRIS, ahead of that planned for CINES in 2020. The number of computing hours available for researchers has been constantly increasing, an absolute essential in maintaining the excellence of our research which needs ever-larger volumes of computing resources for simulating, storing and processing the data being generated, and including Artificial Intelligence dedicated resources.

In addition to these new resources, and following an in-depth review conducted in the closest collaboration with its partners, GENCI was able to finalize its 2019-2023 Strategic Plan, which firmly commits it in the coming years to the road to exascale, reinforcing its positioning inside the European HPC ecosystem.

2019 was itself a very productive year, and these are just the preparations for the next decade.
Editorial by the CEO of GENCI

BY PHILIPPE LAVOCAT

Energy crisis, climate change, GENCI is supporting the scientific community as it works to provide understanding and predictions through the use of numerical simulation enabling the processing of the data generated and providing support in decision making.

In 2019 GENCI adopted its 2019-2023 Strategic Plan: This reaffirms HPC as central in facing our strategic, scientific, social and economic challenges, in a context of the ongoing convergence between HPC, Big Data and Artificial Intelligence. These objectives are positioned in a European context: improvements to existing processes, the evolution of GENCI in its role as a reference solution in response to demands for computing and data processing resources, the diversification of access modes and the integration of partners. This includes the planning for the next stage of the Equip@meso project, coordinated by GENCI.

In response to the AI for Humanity plan of the France’s President of the Republic, Jean Zay, the first converged HPC/AI supercomputer in Europe (16 petaflop/s in 2019, 28 petaflop/s scheduled for 2020), was successfully installed at the CNRS IDRIS center.

GENCI continues its European initiatives, with preparations for the joint-acquisition of an Exascale computer, co-financed by EuroHPC, and the evolution of PRACE into a service provider: Distribution of computing hours, training, technology watch and support for the SME sector. The level of cooperation also has a legal element: GENCI is piloting the procurement procedure for innovative solutions for the PPI4HPC project co-financed by the European Commission, bringing together France, Germany, Spain and Italy. The Joliot-Curie supercomputer at TGCC, integrating the storage resources funded by PIA2, thus received an extension that will increase its performance to over 20 petaflop/s in 2020. GENCI also initiated the procurement procedures for the planned computer at CINES and the storage facilities for CINES and IDRIS.

You will find more details on these areas later in this report.

I would like, in closing, to express my thanks to the team at GENCI for its constant commitment to science, as well as to the teams at the computing centers for their enthusiasm in working for the development of GENCI. Finally, a big thank-you to the Shareholders for the reaffirmation of their confidence as evidenced by the Strategic Plan.

“Scientific advances at the service of knowledge.”
In 2019, the Jean Zay supercomputer enabled the Inria teams to initiate work on mixing HPC and AI. Some of this related to the use of Deep Learning in numeric simulation, using the Melissa software which makes it possible to submit several thousands of instances to a parallel simulation for parametric analyses. Others were related to large-scale studies, for instance for comparing AI algorithms for diagnosing Alzheimer’s disease, or for the systematic evaluation of more than twenty Automated Deep Learning techniques on a hundred datasets. Thanks to Jean Zay, new teams at Inria have made use of GENCI resources, for new uses.

This year again, the work of researchers at CEA was recognized through the HPCwire Prize in the “Best use of HPC in the field of Life Sciences” category, thanks to a PRACE allocation of 24.1 million hours on the Curie computer at TGCC. The Curie computer has now been superseded by the Joliot-Curie supercomputer, launched on June 3, 2019. With the latest extension completed at the end of the year, the computer’s peak processing power was increased from 9.4 to 22.7 petaflop/s and it thus became the most powerful research-focused computer in France. This increase in power takes place in the context of the international competition towards exascale and CEA involvement, alongside GENCI, in the initial actions around preparations for France’s proposal relating to a EuroHPC Exascale computer and its hosting going forward to 2023.
The scheduled replacement of the Ada and Turing computers, alongside the decision, within the AI for Humanity national plan, to integrate a dedicated Artificial Intelligence platform and a donation from Facebook, led to the commissioning last October of the first phase of the “Jean Zay” computer at IDRIS, a “converged” platform with a peak performance of 16 petaflop/s.

The deployment of this new computer is a major event alongside the arrival of a new community at the national centers and the development of specific access modes. This action is perfectly aligned with the strategy of CNRS which aims to provide scientific communities, under the aegis of its Computing-Data Mission, with a response to the inevitable convergence between HPC, Big Data processing and Artificial Intelligence, making full use of the acknowledged and complementary skills of its two national centers, CC-IN2P3 and IDRIS.

2019 was a particularly fruitful year for GENCI and its shareholders, including CPU and the institutions of higher education, research and innovation that it represents. It has positioned this TGIR for the future with the adoption of its 2019–2023 Strategic Plan reaffirming the level of its ambition in terms of the trio of HPC/Big data/AI. One outcome of this during the year was the start of the Jean Zay computer at IDRIS and the Irène Joliot-Curie computer at TGCC, two supercomputers that are now among the most powerful in Europe. This will be followed in 2020 with the renewal of Occigen at CINES, the effectiveness of which was increased in 2019 with the guaranteeing of the availability of its computing capacities for a large number of GENCI’s projects and I would like to take this opportunity to congratulate its teams for their commitment and efficiency.

In achieving this ambition, now more than ever, our institutions will have a key role to play in terms of the initial education of our researchers and engineers of the future. They will be ready to meet this challenge.
HPC and Artificial Intelligence, a necessary convergence

BERTRAND BRAUNSCHWEIG, COORDINATOR OF THE NATIONAL ARTIFICIAL INTELLIGENCE RESEARCH PROGRAM, Inria

Looking beyond the launch of the Jean Zay computer with its computing resources for Deep Learning, I want to highlight here the relationship that is developing between Artificial Intelligence and HPC.

Modern Artificial Intelligence uses enormous volumes of operating data, and requires huge computing resources to accomplish the learning phase. At the same time, modelling and numeric simulation have made remarkable progress over the preceding decades in terms of our understanding of the complex, natural and artificial, systems around us or that we have designed and created.

It would be a tragedy if these two worlds did not interact because they have so much to contribute to each other. Modelling and numeric simulation can make use of automatic learning to help improve the quality of the models used and to calibrate these with observed reality; in return, automatic learning should start from the knowledge we already have of systems and not have to reinvent everything with each new use. We therefore need to know how to make use of all types of models formalizing our best understanding of the systems being analyzed: Numeric models, obviously, but also logic, symbolic, graphic, etc. models.

This convergence is not just desirable for the quality of the modelling and learning, but also quite simply in order to produce significant efficiencies in terms of computing resources and to thus contribute to the better utilization of precious natural resources.

For our country, GENCI is at the very core of these concerns, providing the physical resources for the academic and industrial researchers in these fields to implement this hoped for and essential convergence. The Jean Zay computer, which is beginning to generate these results, is the foundation stone in what is, I hope, an ongoing enterprise when the national exascale computer will be launched to service the connecting of these two research communities.
GENCI’s 2019-2023 Strategic Plan is the result of ten months’ work, including in particular five review sessions with GENCI’s shareholders, a specific working group on partnerships, four pre-Council and Council meeting deliberations. The agreed strategic directions are as follows:

CONTINUATION AND CONSTANT IMPROVEMENTS TO EXISTING PROCESSES

• Be part of the construction of a French research focused ecosystem bringing together in particular data, computing and networks.

• In terms of investment in computers, storage facilities and associated services:
  - Purchase the best possible computers in terms of scientific performances, power-consumption and total cost of ownership;
  - Allocate computing hours to research projects according to the criteria of scientific excellence;
  - Intensify the synergy between the national computing centers;
  - Work with the Technology Watch Unit and COSI (Committee for Strategic Orientation on Investments) in preparing for the future and related investments;
  - Consider the creation of a national system and a process that can be used in certain specific cases to guarantee sovereign purchases.

• Contribute to supporting the growing of the economic competitiveness of French industry.

• Play an active role in promoting numerical simulation.

Evolving role of GENCI

• Set the GENCI TGIR as the reference solution in responding to the computing and data processing needs of public sector research institutions:
  - Adapt to new stakes, new uses and new technologies through the continued diversification of the access modes to computing and data;
  - Undertake a review on the integration of “new partners”.

• Support France’s commitment in the European HPC landscape:
  - Be a part of the implementation of France’s strategy in terms of HPC in Europe namely through the purchase and operation of one of the planned European Exascale computers within the EuroHPC initiative. In this context, GENCI will be the “Hosting Entity” in partnership with the French “Hosting site”;
  - Involvement in the construction of the European ecosystem with the progress of EuroHPC and representation in PRACE.
Large-Scale Research Infrastructure

- p.11_Urbanization, harmonization of services
- p.12_Technology Watch: evolving prototypes
- p.13_New opportunities for users
- p.14_Computing Centres and Supercomputers
- p.18_GENCI events in 2019
- p.20_GENCI in Europe and France
- p.22_Events and Prizes
At the beginning of 2019 it became clear that a number of issues around data needed to be dealt with. We are referring here to storage, transfer, description, etc. Working with the centers, GENCI was able to identify a number of areas for improvement.

The first, relating to CCFR, the very high capacity 10 Gbs network connecting the 3 national centers, was a critical area for the centers as they worked together to ensure its reliability, ease of use and performance.

The second related to the naming, the role and the characteristics of the storage spaces within each center.

It was possible to standardize and rationalize these, thus enabling researchers to move from one center to another with only a minimal impact on their processing chains. This is the final essential stage in the preparations for the introduction of Data Management Plan (DMP) which, within the next few years, all project authors will have to produce when they will ask for significant storage resources. GENCI is working to integrate DMPs into the forms for upcoming DARI campaigns. As part of the “Plan National de Science Ouverte” (National Open Science Plan), this approach is being undertaken in synergy with ANR and CNRS using its OPIDoR tool to accept GENCI DMPs in the future. There are two objectives: To make the writing as easy as possible, and to establish the value of these for researchers and the centers. This therefore requires working very closely with the communities and the hosting centers.

The third relates to new backup, sharing and accessibility services being designed by the joint group of the centers responsible for storage and which should be ready during 2020.

Urbanization, harmonization of services

The urbanization of centers is about developments of the procedures, services and resources available to researchers, to ensure effective support during the actions made possible by GENCI. The objective for GENCI is to facilitate access and use of its computers, regardless of where they are hosted.
2019 was a milestone year for the continuing work on ARM technology with the rolling out at TGCC of a new ThunderX2 ARM technology prototype known as INTI and its opening to the entire scientific community in Q4 2019 (www.edari.fr). An ambition for this platform: To support and work with the French scientific community on the road to Exascale.

The previous two prototypes, Frioul and Ouessant, hosted and operated respectively by CINES and IDRIS were decommissioned at the end of 2019. These had helped scientists to understand and implement the huge changes needed for the new KNL and GPU architectures, which have been deployed in full scale production on the TGCC/CEA and IDRIS/CNRS sites. Mission accomplished.

The INTI prototype was already able to host three hackathons in 2019, enabling those writing the applications to understand the migration process to ARM technology, the scalability of their applications and their sensitivity to ARM SVE, a vectorization feature that will become standard in future ARM processor generations and in particular in the planned European EPI processor, an Exascale candidate.

In addition to its role in making platforms available, the Technology Watch Unit is a vector for sponsoring and accompanying scientific communities in learning about new technologies and their software environments. At the end of 2019, CVT, assisted by TGCC/CEA, AMD and Atos, worked with INP and Coria in preparing a CFD community hackathon on the new AMD Rome platform available at TGCC/CEA. More than 50 researchers, from industry and academia, came together both to build knowledge of the new x86 platform for the AVBP and YALES2 combustion codes and to define new algorithm methodologies for the scientific fields.

2019 was not a slow year, and as for 2020... stay tuned!
This new access, only available on the Jean Zay computer’s dedicated AI section, is intended for researchers looking to develop algorithms, methodologies and tools for AI. A project author must be a permanent member of a research institution, as for any other access to GENCI, but can in this case be a Master 2, Doctorate or Post-Doctorate student in a research institute.

The main objective of this new call is its speed of implementation. It is open throughout the year and can be approved in simply a matter of days. This means there is no need waiting for one of the two annual calls, nor for the several week-long appraisal period. For this access, the two procedures (ressources request and opening the account on the supercomputer) are contained within a single website [www.edari.fr].

In addition, applications for most researchers are, or are in the process of becoming, fully automated. An explanatory video has been produced and can be seen at https://www.youtube.com/watch?v=Marx-BSFMNO and the entire www.edari.fr site has been redesigned to make it even clearer.

In 2020, GENCI will move towards a new type of access known as “Accès de Traitement” (“Processing Access”) which will allow pre or post processing, the analyzing and visualization of the data generated by the computers or intended for the computers without having to submit a computing hours resource request through the bi-annual Regular Access.

As of June 1, on Joliot-Curie, and as of November 1 for Jean Zay and Occigen, GENCI has standardized the mechanisms for managing computing hours at all of the three centers with changes brought to the so-called “bonus” hours. Not only is there no longer a take back of hours but you can now also use and without any specific formalities up to 25% in addition to your annual allocation of hours. A standardized priority system makes it possible to manage the running of work on each computer in a way that ensures this is as fair as possible between projects.
Computing centers & supercomputers

The national computer sources made available to scientific communities by GENCI are hosted and operated in three centers: 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).

JEAN ZAY
16 PFLOP/S HPE SGI 8600 SUPERCOMPUTER
Scalar partition (peak power: 4.9 PFLOP/S)
- Number of computing nodes: 1,528 biprocessor nodes (Intel Cascade Lake, 20 cores, 2.5 GHz)
- Number of computing nodes: 61,120
- Memory per node: 192 GB DDR4-2667 memory (4.8 GB/core)
Converged partition (peak power: 10.7 PFLOP/S)
- Number of computing nodes: 292 nodes including:
  - 261 nodes formed by 2 processors (Intel Cascade Lake, 20 cores, 2.5 GHz) and 4 GPUs (nVIDIA V100, 32 GB memory each)
  - 31 nodes with 2 processors (Intel Cascade Lake 12 cores, 2 GHz and 8 GPUs (nVIDIA V100, 32 GB Memory each) and 384 to 768 GB of central memory
- Number of GPUs: 1,292 V100

OCCIGEN
BULL BULLX SUPERCOMPUTER, 3.5 PFLOP/S
- Total number of processors: 6,732
- Total number of cores: 85,824
- Total distributed memory: 2 to 4 GB/core
- Interconnection network: Infiniband FDR
- 1st level disk space: 5 PB to 100 GB/s with Lustre

JOLIOT-CURIE
BULL SEQUANA X1000/XH2000 SUPERCOMPUTER, 22.7 PFLOP/S
Thin node partition (peak power: 6.9 PFLOP/S):
- Total number of processors: 3,512 (Intel Skylake 8168, 24 cores, 2.7 GHz)
- Total number of cores: 79,488
- Total distributed memory: 4 GB/core

KNL and AMD manycore node partitions
(peak power: 14.7 PFLOP/S):
- Number of processors: 828 (Intel KNL 7250, 68 cores, 1.4 GHz) and 4,584 (AMD Rome 7H12, 64 cores, 2.6 GHz)
- Total number of computing cores: 56,304 (KNL) and 293,376 (AMD)
- Total distributed memory: 64 TB for the KNL partition (1.4 GB/core) and 586 TB for the KNL partition (2 GB/core)

Post-processing partition / AI (peak power: 1.13 PFLOP/S):
- 32 computing nodes with 2 Intel processors for each node Cascade Lake 20 cores, 2.1 GHz and 4 GPU nVIDIA V100, 16 GB
- Total number of GPUs: 128 V100
2019 was a year of renewal for our configurations with Hewlett Packard Enterprise installing the “Jean Zay” supercomputer, which in its first phase includes approximately 71,000 cores, 1,300 latest generation GPUs and 30 PB of storage disks, with a peak power of 16 PFlop/s. As well as conventional numeric modelling applications, some of which will benefit from the increased power of the accelerators (at the initiative of GENCI, six emblematic HPC applications created by French communities have already been successfully migrated to GPU by the teams at IDRIS and HPE), this platform is also the first at the national level dedicated to research into Artificial Intelligence and it is furthermore the first configuration that allows converged uses of numeric simulation and Artificial Intelligence.
Following the installation and start of production on Joliot-Curie Phase 1 in 2018, in 2019 the teams at TGCC set about moving on to Phase 2, financed by GENCI and the European PPI4HPC project. Two new computing and post-processing partitions were thus added to Joliot-Curie. The first included 2,292 computing nodes (AMD Rome Epyc 2.6 GHz bi-processors with 64 cores per processor), and for the second, 32 hybrid nodes (each node with 2 Intel Cascade Lake 20 core 2.1 GHz and 4 Nvidia V100 GPU processors). The Joliot-Curie supercomputer now offers its users 4 different types of computing and post-processing partitions.

This latest phase for Joliot-Curie has been deployed, in software terms, thanks to the new “OCEAN” administration software stack, developed by CEA/DAM/DSSI. This makes it possible to optimize the deployment of the computing nodes, leading to greater flexibility and efficiency during the integration of future computing partitions or future software updates. This environment will facilitate the optimized management of heterogeneous computers, such as the future exascale computers.

The AMD extension was opened on schedule to the “Grands Challenges” at the beginning of December 2019. The GPU extension will be open from the beginning of January 2020. Twenty-five Grands Challenges, including 2 on the GPU partition, will thus be sharing the Joliot-Curie supercomputer resources (“Rome” and “V100” partitions) until April 2020 for the “Rome” part, and October 2020 for the “V100” part. The teams at TGCC and Atos are making their expertise available to these pilot users whilst maintaining an optimal level of production on the rest of the configuration and services.
Large-scale Research Infrastructure

640 million computing hours were used on the Occigen supercomputer in 2019, with an excellent utilization rate of 86% for a computer that has now been in production for 5 years.

2019 was also the year of Europe at CINES with two large new projects in the computing and data fields: the PHIDIAS project (https://www.phidias-hpc.eu), for the creation of innovative HPC/HPDA services, and the EOSCPillar project (https://www.eosc-pillar.eu), to coordinate national initiatives around open science and make progress on the FAIRisation of research data. With the arrival of Big Data in the HPC world, this is shaking up the way things are done in computing centers as they now need to provide services that are comprehensive and easily usable for storing, processing and finally for distributing the huge volumes of data generated through observations, experiments and the numerical simulations.

In partnership with the Data Terra research infrastructure, which supplies spatial big data from the Earth system, PHIDIAS is an initial pilot for the deployment of integrated HPC/HPDA services that will eventually form the building blocks for the future CINDI (CINES Data Infrastructure).
2019 highlights

Inauguration of French Joliot-Curie supercomputer, dedicated to French and European research

French third supercomputer, Joliot-Curie, starting at 9.4 petaflop/s, as of 2020 is now the most powerful research-dedicated supercomputer in France, with a peak power of 23 petaflop/s. Designed by Atos, a European leader in supercomputing, for Grand Équipement National de Calcul Intensif (GENCI), this newest computer, hosted at CEA TGCC (Très Grand Centre de Calcul), was inaugurated on June 3 2019 by François Jacq, CEA General Administrator, Thierry Breton, Atos CEO, and Philippe Lavocat, GENCI CEO.

LARGE-SCALE RESEARCH INFRASTRUCTURE

In 2019, the computing power of Joliot-Curie has been more than doubled in 2020. This will in effect reach 23 petaflop/s, i.e. 23 million billion operations a second, thus making it the most powerful research supercomputer in France. This raising of the computing power of the Joliot-Curie supercomputer is part of the international exascale competition, which aims to reach a computing power of one billion of billion operations a second, representing a strategic challenge in terms of the competitiveness of the actors in the digital economy.

Thanks to the investment by GENCI, Joliot-Curie also allows France to fulfill its commitments in terms of computing power made available to European researchers in the context of the PRACE2 European computing infrastructure.

AN ANTICIPATED TOOL AT THE SERVICE OF SCIENTIFIC AND INDUSTRIAL RESEARCH

The areas of application for supercomputers are extremely varied, allowed the advances being made in terms of these computers making it possible to extend...
numerical simulation to all disciplines. The “Grands Challenges”, organized by GENCI at TGCC, have already tested Joliot-Curie by running large simulations and a variety of applications.

The use of numeric simulation and HPC is now an essential scientific tool, in increasing our knowledge, in design work and decision-making, in the fields of fundamental and applied research as well as in an increasing number of industrial sectors.

CEA’s Très Grand Centre de Calcul (TGCC), a high performance scientific computing infrastructure, located in Bruyères-le-Châtel (Essonne), now hosts, alongside Cobalt, an industrial focused supercomputer, the new Joliot-Curie computer, being made available for research requirements. The Joliot-Curie computer is currently being used for more than fifteen fields including the climate, astrophysics and geophysics, biology, molecular dynamics and materials properties and, in the near future, genomics, neurosciences...

---

**Expo BIS at La Sorbonne**

As part of its mission to promote HPC within new communities of users, GENCI launched its “10 years of HPC” exhibition in 2017. This exhibition became a roadshow in 2018 in order to take it to users in the regions and thus reach a new public audience. In 2019, the focus was placed on the Human and Social Sciences (HSS) community with a workshop and a poster exhibition at La Sorbonne between April 4 and June 28, 2019. The workshop was held on April 16 in the presence of researchers from a range of HSS subjects: geography, archeology, language decoding, social networks. Presentations highlighting the value of HPC and numeric simulation for the HSS community enabled them to understand how to make use of these resources and tools. The exhibition was completed with HSS dedicated posters created with the support of the regional computing centers:

- **Observation of an archeological society**: the trajectory of the LBK Neolithic. OBRESOC team, J.-P. Bocquet-Appel.
- **Fighting the emergence and spread of DENGUE**: E. Daudé et al. UMR 6266 Laboratory CNRS, Rouen Normandie University.
- **Simulation of fiscal policy**: L. Stimula, GATE Laboratory, ENS Lyon, UME 5824
- **Classification of Twitter users on the basis of their behaviors**: V. Brault et al. PACTE, LJK, GRESEC, Grenoble Alpes University.
- **Assessing the esthetic quality of the countryside**: Y. Sahraoui, G. Vuidel, ThéMA CNRS Laboratory / Franche-Comté University.

---

**HPC Exhibition in Nantes**

As part of the Festival of Science, the School’s centenary celebrations, as well as the 4th anniversary of its computing center, Centrale Nantes hosted the exhibition between September 26 and October 7. The ICI computing center joined the Equip@meso network in 2019. GENCI was proud to be able to help facilitating this exhibition with its new partner and thus helping promote HPC in the Pays de la Loire region.
GENCI in Europe and in France

PRACE-5/6IP European Projects and CEF AQMO

The year saw the transition from PRACE-5IP to its successor PRACE-6IP (INFRAEDI-01-2018), a 32-months project with 26 partner countries, being coordinated by JSC (Jülich) on behalf of PRACE Aisbl, with its kick-off meeting in Bratislava in May 2019. The challenge facing it is to provide an integrated solution for the HPC needs of academic and industrial researchers, taking into account the evolution of the European ecosystem and its three pillars (ETP4HPC (technology), Centers of Excellence (applications) and PRACE (infrastructure)), EOSC (European Open Science Cloud, access portal to digital services for open research in Europe), EPI (European Processor Initiative), and above all EuroHPC.

GENCI is also involved in the AQMO “smart city” project (CEF-TC-2017-3 Connecting Europe Facilities). This, alongside its environmental science component (enabling better access for authorities and citizens to air quality data), allows the testing of innovative access modes to HPC resources, with a continuum from the instrument systems (IoT / Edge computing) to the computing center, in the search for new uses of EuroHPC resources. The consortium is being coordinated by IRISA, and consists of IDRIS, several SMEs (AmpliSIM, UCit, Ryax, Neovia), Keolis (bus operator), AirBreizh (air quality) and Rennes Métropole authority.
The extension of the activities of the EuroHPC initiative, launched at the end of 2018 by the European Commission and 32 Member States, again continued during the year. This included a first call for projects around the development of hardware and software technologies for HPC and data, as well as support for industrial users through Competences Centers.

In terms of infrastructure, EuroHPC announced the co-financing of multi-petascale systems in Bulgaria, Portugal, Luxembourg, Slovenia and the Czech Republic available as of the end of 2020 and selected 3 hosting sites (Finland, Spain and Italy) for its pre-Exascale systems available in 2021.

For the allocation of computing cycles on the computers, as well as the provision of training and support services, EuroHPC is focused on PRACE which is currently preparing a service package, PRACE3, scheduled for early 2021.

---

**EuroHPC – PRACE increasing interconnection**

Official signing ceremony between EuroHPC and its partners for the multi-petascale and pre-exascale systems (26 Nov 2019).

---

**Equip@meso bows out**

Equipex Equip@meso came to its end on 31st December 2019. Started in 2011 in the context of the Projets Investissement d’Avenir (PIA1), the project enabled 10 regional computing centers to equip themselves with more powerful computers. The total regional power was thus increased from 0.4 petaflop/s in 2011 to 1.33 petaflop/s in 2013 (end of the investment phase).

Seven Mésocentres have joined the network since 2013. The total computing power for the 17 Mésocentres will thus reach 10 petaflop/s in 2020.

The Mésocentres contributed to actions organized around three working groups: Tier1-Tier2 Link, coordination/training and SiMSEO.

As part of the Tier1-Tier2 Link group, they were equipped with PerfSONAR sensors to enable them to measure the data flows between centers. The initiatives were coordinated by CRIANN, together with RENATER. There were also visits by delegations to SuperComputing (HPC specialized conference) during the years 2013 and 2018, to allow the Mésocentres to discover what the equipment makers were developing and consider extensions to their computers.

Promotional events, focused scientific days and hackathons were held to keep user communities informed about new technologies and scientific advances throughout the project. Prizes were awarded each year to academic and industrial researchers for their outstanding work through the Mésochallenges days. These events were linked with the Mésocentres days of the Computing group and the GIS FRANCE GRILLES of GRID’5000 and GDR RSD SUCCES days in 2018 to form the JCAD bringing together the whole of the regional HPC community.

Finally, SiMSEO is the project to support the SME sector into modelling and numerical simulation. The project was created in 2015 in the context of PIA 2 with 6 volunteer Mésocentres. This has so far helped to reach and increase awareness among 1,800 companies.
In 2019, GENCI took part in a number of national conferences such as Teratec and AI Paris, as well as other international events. A first: GENCI was present at the VivaTech fair, the international meeting place for startups and innovation, in partnership with HPE, to introduce Jean Zay, its brand new supercomputer!

GENCI MAKES ITS FIRST APPEARANCE AT VIVATECH

In May, in Paris, at the VivaTech global summit for startups and leaders in innovation, GENCI was in an HPE dedicated corner, on one of the largest and most popular stands at the fair, with specific sessions designed for startups, the press and the general public.

ISC - JEAN ZAY JOINS THE TOP500

The Jean Zay supercomputer joined the Top500 (world ranking supercomputers) officially in June 2019 during ISC, the European HPC trade fair, held in Frankfurt, Germany. In its 42nd ranking in the Top500, it also joined the Top3 most powerful supercomputers in Europe in the category of converged open research accessible computers.

SUPERCOMPUTING SC19

As every year, GENCI was present on the CNRS stand, alongside the IN2P3 and IDRIS computing centers.

GENCI announced a boosting of the computing power of Jean Zay, from a peak of 14 petaflops to 16 petaflops as of the end of 2019. In effect, with the announcement by Facebook of a grant of $3M during the TechForGood conference in 2018, GENCI was able to finance and install 31 additional servers, with particular benefits for the Artificial Intelligence community, as part of the Government’s “AI For Humanity” plan. Each node is 8 GPU NVIDIA V100 32 GB, with a memory capacity from 384 to 768 GB and local inputs-outputs in addition to the global storage capacities. This made it possible...
to increase the number of GPUs initially installed on the supercomputer by 25% (giving a total of almost 1,300 GPUs).

GENCI also presented the extension to Joliot-Curie which had been financed as part of PPI4HPC, the joint European procedure for purchasing innovative computing technologies. These new AMD EPYC™ 7H12 Series chip equipped BullSequana XH2000 computing and post-treatment/AI partitions increased the power of Joliot-Curie from 9.4 to 23 petaflop/s. These processors stood out as they set new world records in terms of server performance, as well as in energy consumption thanks to the "Enhanced Direct Liquid Cooling system". GENCI is proud to have been the first in the world to make these AMD EPYC™ 7H12 Series processors available, as of November 2019, to the French and European scientific communities.

Denver, 20th November – The “HPCwire Readers’ and Editors’ Choice Award” in the “Best use of HPC in Life Sciences” category was awarded to CEA at SC’19 (The International Conference for High Performance Computing) held in Denver, Colorado, for its use on a GENCI computer within the PRACE infrastructure. Tom Tabor, CEO of Tabor Communications, editor of HPCwire, presented the prize to the representatives of GENCI (Philippe Lavocat - CEO), CEA (Jacques-Charles Lafoucrière - Director), and PRACE (Serge Bogaerts - Managing Director), on the PRACE stand.

The French research team headed by Luc Bergé, Director of Research at CEA, obtained a PRACE allocation of 24.1 million hours on GENCI’s Curie supercomputer (hosted at TGCC, CEA, France) for the CAPITOL project to explore, by means of various massively parallel codes, new physical mechanisms converting ultra-intense laser light into photons and particles ranging from terahertz to X-rays and including laser-plasma interactions, potentially leading to a breakthrough in breast and skin cancer tumor detection.
2019 was the year in which the new Jean Zay supercomputer was launched at IDRIS. Its opening to the community with the A7 Call helped relieve the ever-increasing pressure on the Joliot-Curie SKL computer. It was the cooperation between the Chairs of the Thematic Committees, the Directors and users of the Centers that once again proved decisive in optimizing computing resource allocations across the various computers at the centers to ensure most efficient use of limited national resources.

Training and coordination for applications are major challenges arising from new architectures and Europe’s ambitious plans in terms of HPC.

The end of Moore’s Law means there is an increasing need for coordination for applications in order to achieve the best possible performances for the computers. These needs and the ways to meet them were the subject of discussions between the Chairs of the Thematic Committees, representatives of the users, Center Directors and GENCI. These meetings highlighted the importance and the quality of the application support from the centers and the training needed. The difficulties experienced by research teams in terms of code optimization because of a lack of skills in optimization and also in many cases a lack of appreciation of this work were identified.

In order to best distinguish the requirements of the various communities and test the performances of new architectures, a set of benchmarks, shared across all centers, has also been compiled in liaison with the Thematic Committees. Given the new architectures and Europe’s ambitious plans in terms of HPC, coordination of applications has become an increasingly critical challenge.

SYLVIE JOUSSAU ME, CHAIR OF GENCI’S EVALUATION COMMITTEE
**Thematic Committees, forewords of the Chairs**

**CT1**

**Environment**

GERHARD KRINNER, CHAIR OF CT1

Most of the projects of CT1 “Environment” concern the climate system as a whole and its components (ocean, atmosphere, continental surface, ice, biogeochemical cycles). A smaller number of the projects in this CT deal with environmental issues as such, in the sense of dispersal of pollutants at sea or in the atmosphere. The current and foreseeable technical evolution of the computer remains a challenge for our community. In 2018 and 2019, our community has been strongly mobilized for climate modelling projects related to the work of the IPCC. Usually pluriannual, the many high quality projects that we have evaluated this year are mostly carried out in a framework of European and global collaborations.

**EVELYNE RICHARD, CHAIR OF CT1 (1ST PERIOD 2019)**

**CT2a**

**Non-reactive and multiphase**

GUILLAUME BALARAC, CHAIR OF CT2a

The simulation of flows covers a wide range of activities, from fundamental analysis to technology transfers. The 71 projects this year highlight this diversity, with proposals aimed at increasing our understanding of turbulent flows and 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 2019, 46 projects submitted to CT2b received CPU time on GENCI’s supercomputers, among these projects 15 were new projects. The range of the research topics addressed by CT2b is extremely large, since it includes all flows being reactive or multiphase. The experts thus evaluated projects on topics such as atomization in diphasic flow, combustion instabilities in rocket engines, decarbonated energy production, biological flows or detonations. The vast majority of the software developed performed extremely well no matter what the computer architecture. This enabled flexibility concerning the allocation of requested CPU time on the various supercomputers, alleviating the very high level of pressure on some of the supercomputers.

**CT4**

**Geophysics and astrophysics**

FRÉDÉRIC BOURNAUD, CHAIR OF CT4

CT4 this year considered an even larger number of projects, with applications in many cases requesting very large amounts of computing time on GENCI’s supercomputers. Geophysics projects continue to expand in terms of scope, and astrophysics projects apply ever-increasing amounts of computing power for their multi-scale studies. A large number of the new studies are based around the use of innovative approaches: artificial intelligence applications, simulation emulation on GPU, modeling of space instrumentation, etc.

**CT5**

**Theoretical physics and plasma physics**

ERIC SERRE, CHAIR OF CT5

With 40 projects and around 260 million CPU hours, theoretical physics and plasma physics were again major users of HPC in France in 2019 (12% of allo-
cated resources). The projects were scientifically and technically outstanding with 30 projects rated AA. The main topics remained the QCD, high-intensity laser/matter interaction, and fusion by magnetic confinement. Whilst projects using supercomputers based on standard CPU remain in the majority, an increasing number have migrated totally or partially to new processor architectures (7 projects using XeonPhi and GPU). At the same time, in order to meet increasingly high performance requirements, large projects with more than 10M hours (9 in 2019) are organized around key community codes developed for the scientific discipline (GYSELA, SMILEI, CALDER, JOREK, TOKAM3X, XTOR, etc.).

CT6
Computing, algorithms and mathematics

DIDIER AUROUX, CHAIR OF CT6

The projects evaluated by CT6 range from numerical algorithms to parallelization problems: Resolution of large linear systems, development of libraries, scalability studies, schemes adapted to parallelization, etc. Some projects require large volumes of hours to build a database from the numerical simulations in various configurations in order to build reduced models. The new hybrid architectures seem perfectly adapted for those problems that combine HPC and AI.

CT7
Molecular modelling applied to biology

MARC BAADEN, CHAIR OF CT7

In 2019, the CT7 committee reviewed around 30 proposals per call, with a roughly equal distribution between the two calls. All-atom or coarse-grained molecular dynamics (MD) were central in these. Many projects related to simulations of proteins interacting with various partners (ligands, co-factors, etc.) and attempted to understand the role of dynamics with respect to the function of these biomolecules. GENCI resources enable simulations of systems of considerable size and allow the explicit inclusion of an environment, such as an aqueous solvent, a lipid bilayer (etc.), to achieve as realistic as possible simulations. This year the availability of a GPU partition on the Jean Zay machine aroused keen interest in this committee for this architecture. GPUs that make it possible to capitalize on recent MD code versions such as GROMACS, NAMD and AMBER-GPU, that are finely tuned for these architectures.

CT8
Quantum chemistry and molecular modelling

DAVID LOFFREDA, CHAIR OF CT8

These project application domains cover a wide spectrum of areas of interest in chemistry, physics and biology, and we have seen the emergence of a considerable number of studies of reactive interfaces, in a general sense. The systems described are also more and more complex and realistic in terms of experience, and thus the demand for computing time has increased significantly year-on-year. The CT8 research community consists of developers, code contributors, as well as the users. Interaction with application support from the three GENCI centers is thus essential, in particular for the porting of all the quantum chemistry codes for the new Jean Zay computer at IDRIS and Rome AMD at TGCC. The Committee would like to thank them for their technical support.

CT9
Physics, chemistry and materials properties

THIERRY DEUTSCH, CHAIR OF CT9

CT9 appraised 103 proposals with an average request for 1.8 million computing hours. The increase in computing capacity means that, unlike last year, there has not been any penalizing of the ab initio molecular dynamics projects that are the most greedy in computing time. We also note the emergence of a number of projects using machine-learning techniques to replace computationally intensive steps that are heavy users of GPUs for the learning phase.

CT10
New applications and multidisciplinary applications of HPC

BRUNO SCHEURER, CHAIR OF CT10

CT10 evaluated 12 proposals, for a total allocation of 32 million hours. These projects covered fields such as nuclear reactors, planet mineralogy and electromagnetism. It is also worth noting that in 2019 the fields covered by the Committee were extended to include Artificial Intelligence. Thus, the ‘Grand Challenges’ campaign (for Jean Zay) and the dedicated AI portal, were the subject of many of the proposals.

IMPACT OF GENCI FOR THE SCIENTIFIC COMMUNITY
2019 main scientific results

The scientific results outlined in the pages below have been produced through research work carried out in 2019 using the computing resources provided by GENCI. Whilst these projects are representative of the various scientific domains making use of the national supercomputers, they are however only a sample of the 564 projects that were allocated computing time in 2019. To find out about other results, you can visit: www.genci.fr

29. Theoretical physics
   CT5: Explaining the measurement of the magnetic moment of the muon

30. Earth and astro sciences
   CT1: Climatic variability and climate change
   CT4: Extreme stellar explosions: from magnetic field amplification to the launch of the explosion

32. Fluid mechanics
   CT2a: Understanding the flow in nuclear fuel assemblies
   CT2b: Simulations of a solar calcination reactor with a gas-solid fluidized bed

34. Biology, chemistry and materials
   CT9: Screening effect in 2D materials
   CT8: Massively parallel quantum chemistry
   CT7: Structural dynamics linked to mutation-associated protein activation in cancer

37. Other applications
   (computing, health, etc.)
   CT3: Deciphering the mechanisms of action of the G protein-coupled receptors
   CT6: Study of Navier-Stokes 3D time discretization strategies on the efficiency of parallelization in PETSc
   CT10: Pl@ntNet addresses the problem of the recognition of the world’s flora
Theoretical physics

CT5 THEORETICAL PHYSICS AND PLASMA PHYSICS

Turing © 100,000,000 hours (with additional resources from FZ Jülich, Leibniz Supercomputing Centre München, High Performance Computing Center Stuttgart)

Is a new fundamental physics needed to explain the measurement of the magnetic moment of the muon?

Budapest-Marseille-Wuppertal collaboration -- CNRS, Aix-Marseille U., U. de Toulon, CPT, Marseille, France; Bergische Universität Wuppertal, Germany; Forschungszentrum Jülich, Germany; Eötvös University, Budapest, Hungary

LAURENT LELLOUCH, DIRECTOR OF RESEARCH CNRS, CENTRE DE PHYSIQUE THÉORIQUE, CNRS, AIX-MARSEILLE UNIVERSITY, UNIVERSITY OF TOULON

The Standard Model (SM) of particle physics, which provides a quantum description of all known subatomic particles, was one of the great scientific achievements of the 20th century. Despite this, there are observations and theoretical features of the model which suggest that it cannot tell the full story. Thus, scientists around the world are searching for clues for what may lay beyond. One approach consists of measuring properties of elementary particles with extreme precision and in comparing these measurements with equally precise calculations in the SM: Any significant disagreement would signal the discovery of new fundamental physics.

A particularly interesting property relates to the muon, a short-lived cousin of the electron. As any elementary particle that spins, the muon behaves like a tiny magnet that is characterized by a magnetic moment. Currently this magnetic moment is measured and predicted with a relative precision of around $6 \times 10^{-10}$! Experiment and theory are more than 3 standard deviations apart, still too little to fully determine the fate of the SM. There is however a new experiment underway aimed at reducing the measurement error by a factor of 4 over the next 2 years. If the SM prediction can be similarly improved and makes the disagreement even more significant, a new fundamental physics will have been discovered.

It is in this context that our team is performing an ab initio calculation of the contribution that is most limiting on the precision of the SM prediction for the muon magnetic moment. This contribution is due to highly non-linear effects of the strong nuclear force that cannot be computed with pen and paper. Its calculation requires solving the equations of Quantum Chromodynamics with, in the order of, $10^9$ variables. Thanks to the work of scientists from around the world, massively parallel supercomputers, such as IDRIS’ Turing, can be used very effectively to undertake such challenges.

Current status of calculations of the hadronic vacuum polarization contribution to the magnetic moment of the muon. GENCI’s 2018 and 2019 allocations should allow us to reduce the uncertainties of our BMWc 17 results by a factor of around 4 and to unambiguously confirm or refute the current disagreement between theory and experiment — distance between points labeled “phenomenology” and the center of the vertical green band.
Earth and astro sciences

Climate variability & climate change

IPSL Climate modelling centre (https://cmc.ipsl.fr)

OLIVIER BOUCHER, DIRECTOR OF RESEARCH, CNRS AND RESEARCHER, LABORATOIRE DE METEOROLOGIE DYNAMIQUE (LMD-IPL, CNRS/UPMC/ENS/ECOLE POLYTECHNIQUE)

Climate models can be used to simulate current and future warming due to human-induced greenhouse gases. Particular attention is paid to the recent period from 1850 to the present because it is relatively well observed and can serve as a testbed for models. However, the interpretation of the results is complicated by the fact that the climate system has evolved both because of natural internal processes (internal variability at interannual, decadal and even multi-decadal scales) and in response to perturbations of natural (volcanic eruptions in particular) and anthropogenic origin (increase in greenhouse gases, change in concentrations of particulate pollution).

The IPSL Climate Modelling Centre was able to carry out not one but thirty-two simulations of the 1850-2018 period, which differ only by their initial conditions in 1850. This “grand ensemble” of simulations makes it possible to separate internal climate variability from the long-term trend. The first figure shows the change in the global-mean surface temperature relative to 1850-1899 for each of the 32 simulations.

The average of the simulations corresponds to the «forced» component of the climate in response to the perturbations, and variations around this average represent the effects of internal climate variability. The model shares a number of characteristics of the observed temperature change in terms of long-term trends, response to volcanic eruptions (Krakatoa, Pinatubo), and internal variability with the existence in some members of relative “pauses” in the warming. The second figure illustrates how trends over a relatively short period (1998-2018) vary among 16 different members in comparison to observations. Climate models allow us to better interpret and understand the recent climate, but also to anticipate future changes according to different socio-economic scenarios. Results from these simulations will be analysed along with those from other models to be incorporated in the next IPCC report scheduled for 2021.
Earth and astro sciences

CT4 ASTROPHYSICS AND GEOPHYSICS
Occigen 6.5 million hours / Joliot-Curie 4.5 million hours

Extreme stellar explosions: from magnetic field amplification to the launch of the explosion

Département d’Astrophysique, IRFU, CEA Saclay

Stellar explosions, such as supernovae and gamma-ray bursts, are important events in astrophysics because they have a decisive impact on their environment, in particular through their feedback on stellar formation and for the nucleosynthesis of heavy elements. One of the most likely scenarios to explain the most extreme of these explosions consists of the formation of a magnetar (a class of very magnetized neutron star whose dipole magnetic field is of the order of $10^{15}$G) rotating rapidly with a period of the order of a millisecond. However, this scenario has not yet been confirmed, in particular due to a lack of predictive theoretical models because the origin of the magnetic field is poorly understood.

Within the framework of an ERC project called MagBURST, our team is endeavoring to understand the physics of the magnetic field amplification when a neutron star forms and to use this understanding to improve explosion models. For this purpose, we have adapted the numerical methods used to study planetary and stellar dynamos for this context.

Our allocation on the Occigen and Irene computers allowed us to develop the first simulations of a convective dynamo in a nascent neutron star. These have revealed the appearance of a new dynamo branch giving rise to extremely intense magnetic fields of $10^{15}$ to $10^{16}$G if the rotation is fast enough (see Figure). These results are compatible with the observational constraints on magnetars observed in the galaxy and are very promising for models of extreme explosion. In addition to these simulations centered on the interior of the neutron star, we have developed simulations of the explosion generated by the birth of a magnetar. These notably highlighted the importance of correctly describing the geometry of the magnetic field to predict the properties of the explosion.

Left to right: MATTEO BUGLI, JÉRÔME GUILET, RAPHAËL RAYNAUD, ALEXIS REBOUL-SALZE, DÉPARTEMENT D’ASTROPHYSIQUE, IRFU, CEA SACLAY

Simulation of a convective dynamo in a protoneutron star. Magnetic field lines are colored by the total field strength, which is of the order of $10^{15}$ G. Blue (red) isosurfaces of the radial velocity represent the downflows (outflows).

3D visualisation of a magnetorotational explosion with a quadrupolar magnetic field. The magnetic field lines are colored according to the intensity of the magnetic field.
The numerical analysis of the flow in a nuclear reactor core must take into account a wide range of geometrical scales that can influence the thermal efficiency of the reactor. An 1100 MWe nuclear reactor core for example may contain 193 fuel assemblies. Each fuel assembly consists of 17×17 fuel rods. Up to 10 mixing grids are present in a fuel assembly for mechanical reasons to maintain the rods in place and for thermal-hydraulic reasons to improve the thermal efficiency.

To increase the thermal exchanges between fuel rods and coolant, small mixing vanes just a few millimeters long are located at the top of the mixing grids to increase the turbulence level and to initiate cross-flows. Fig.1 shows the multitude of geometrical scales by zooming from the whole nuclear reactor to the mixing vanes.

In order to predict the flows in fuel assemblies, a calculation methodology was developed at CEA that is based on the open source code TrioCFD, a general CFD code developed at CEA-Saclay. The flow in parts of one fuel assembly and of clusters of 2×2 assemblies were analyzed. The calculations show that the control rods, which are present in each fuel assembly to pilot the power of the reactor, significantly hinder the formation of cross flows. The influence of the width of the gap between two adjacent assemblies on the inter-assembly exchanges was quantified. It was also possible for the first time to define the self-stabilizing horizontal force that helps to maintain this gap width. Fig.2 shows the cross flows in a cluster of 2×2 assemblies, which are reduced in the gaps between the fuel assemblies (see zoom to the center of the cluster).

These complex geometries were simulated using 500 million tetrahedral meshes. These calculations used 8,960 processor cores on the OCCIGEN (CINES) cluster.
Simulations of a solar calcination reactor with a gas-solid fluidized bed

Laboratoire PROMES-CNRS (UPR 8521)

ADRIEN TOUTANT, SENIOR LECTURER HDR, UNIVERSITE DE PERPIGNAN VIA DOMITIA (UPVD)

The objective of the solar calcination research is to study solar receiver/reactor concepts for the thermal treatment of reactive particles in the energy-intensive non-metallic mineral industries, such as the treatment of cement, lime, phosphate or clay. These industries, which are the second largest energy consumers and CO₂ emitters (after the energy industry), need most of their energy input as the heat and this is currently provided by combustion. As part of the H2020 SOLPART project, a horizontal compartmentalized fluidized bed reactor was successfully tested at the focus of the 1000 kW solar furnace in the PROMES laboratory for dolomite decomposition.

The device was modeled and simulated with the NeptuneCFD software on the Occigen supercomputer. The model used applied the Euler-Euler approach. The dispersed phase is considered as a continuous medium. Solid particles are represented by a presence rate. The performed simulations are three-dimensional and unsteady. In the long term, they should help in increasing the pilot scale to an industrial scale. To do this, the analysis and processing of simulation data allows:

- The study of the strong couplings between velocity, temperature and chemical reactions. One of the important phenomena of reactors is the degassing of particles during their calcination (thermal decarbonation). This degassing phenomenon can modify the fluidization rate and therefore the fluidized bed regime.
- The selection of particle size, temperature and residence time control of particles which are major challenges in the development of industrial reactors.
- Information for more macroscopic models such as the bubble-emulsion model or RANS simulations (stationary).
The excitation of valence electrons is at the origin of the optical absorption, or electron energy low loss spectra. These quantities result from the dielectric properties of the material, which express its capability to screen the perturbation.

In solid state physics, crystals are modeled as 3-dimensional (3D) periodic structures, which enables the large efficiency of reciprocal space computer codes. Ab initio formalism is the state-of-the-art. The appearance of nano-objects like graphene, nanotubes, etc., allows the emergence new properties, arising from the quantum confinement and the modification of the screening. To describe a nano-object in the framework of reciprocal space codes, one uses a supercell where the object is embedded in a vacuum to isolate it from the replicas inherent to the periodic formalism. A surface is modeled by a thick slab inside a supercell with a vacuum in the perpendicular direction. Within the ab initio formalism of Time-Dependent Density Functional Theory (TDDFT), we have shown that the use of a supercell gave non-physical results depending of the thickness of the vacuum.

We have shown that the equation of TDDFT should be solved in a subspace of reciprocal space vectors defined according to the thickness of matter. This method, called Selected-G, provides spectra independent of the choice of the supercell, maintaining the efficiency of reciprocal space codes. During this derivation, we have obtained a new expression for the effective Coulomb potential in reciprocal space, called slab potential. In the limit of a thick slab, one again finds the expression of the 3D Coulomb potential. In this limit, the Selected-G method allowed us to simulate the absorption of a surface of silicon for the 3 directions of polarization. Using the slab potential, we have reproduced the pioneering experiments of electron energy loss of slabs composed of 1 to few layers of graphene. These results are crucial in calculating quasiparticle correction or excitonic spectra of nano-objects.

This work benefited from computing time on supercomputers Ada (IDRIS) and Irene (TGCC) and led to the publication of 3 publications in Physical Review B.
Massively parallel quantum chemistry

Laboratoire de Chimie et Physique Quantiques, Toulouse

Our research project focuses on the development and application of massively parallel numerical methods for solving the electronic Schrödinger equation which is at the heart of chemistry. A first line of research concerns the development of a Quantum Monte Carlo (QMC) method based on a probabilistic interpretation of the Schrödinger equation. In practice, quantum properties are expressed as time averages along independent stochastic trajectories of electrons, an ideal situation for parallel computation since these trajectories can be run independently on an arbitrarily large number of computing cores. Thus, thanks to the GENCI supercomputers, several important physicochemical problems have been solved in recent years. For example, a “grand challenge” organized by GENCI a few years ago on the Curie supercomputer demonstrated the possibility of using all the computing cores of the machine (nearly 80,000) to compute relevant chemical quantities for a peptide of medical interest. A second line of research concerns the development of a massively parallel version of the more traditional deterministic quantum chemistry algorithms (configuration interaction methods). We have shown that, contrary to a common idea, these equations can also be processed by massively parallel computers, in particular by using an original “probabilistic/deterministic” hybrid algorithm developed in our group. This unique implementation of configuration interaction methods led to the development of a general-purpose quantum chemistry software, Quantum Package (https://quantumpackage.github.io/qp2/).

A very good scalability (up to more than a dozen of thousands of compute cores) has been demonstrated thanks to the support of GENCI. This code is currently used and developed by several groups in France and abroad.
Structural dynamics linked to mutation-associated protein activation in cancer

Roland H. Stote, Séverin Vanthong, Kays Al Badawy, Annick Dejaegere
Département de Biologie Structurale Intégrative, Institut de Génétique et de Biologie Moléculaire et Cellulaire (IGBMC), Institut National de La Santé et de La Recherche Médicale (INSERM), U1258/Centre National de Recherche Scientifique (CNRS), UMR7104/Université de Strasbourg, 67404 Illkirch, France.

Nuclear receptors (NRs) are a superfamily of ligand activated transcription factors. The binding of ligand by NRs leads to the recruitment of coactivator proteins that subsequently lead to the recruitment of the gene transcription machine. NRs are complex allosteric modulators that contain several domains, including a DNA binding domain and a ligand binding domain. NRs are involved in the transcriptional regulation underlying many physiological and, by extension, pathological processes. As a result, they are major pharmaceutical targets. Nuclear receptors can exhibit anti-tumor or pro-tumor activities.

Our project focused on the Peroxisome Proliferator-Activated Receptor gamma receptor (PPARγ), an important target in many diseases including diabetes and cancer. Our collaborators at the Institut Curie have associated an alteration of the PPARγ gene with a particular subgroup of differentiated luminous tumors that represent 50% of invasive muscle bladder tumors. Our project studied the ligand binding domain of wild-type forms with mutation-forms of PPARγ associated with bladder cancer. Experimental tests showed that some of these mutation receptors induced a higher transcriptional activity observed in the wild-type. We used molecular dynamics simulations to study the impact of these activating mutations on the structural dynamics of the receptor. We have shown that mutations lead to a stabilization of the ligand binding domain and promote interaction with coactivating peptides, an interaction critical for the induction of gene transcription.

Our calculations made it possible to make the link between changes in the structural dynamics and the increased transcriptional activation of the mutated forms of PPARγ identified in tumors. This collaborative work was published in Nature Communications 2019 10: 253.
Deciphering the mechanisms of action of the G protein-coupled receptors

Laboratoire MITOVASC, UMR CNRS 6015 – INSERM U1083, ANGERS

MARIE CHABBERT, CNRS - SENIOR SPECIAL RESEARCH FELLOW

The 800 human G protein-coupled receptors (GPCRs) are transmembrane receptors that transduce information from the outside to the inside of a cell. They participate in numerous important physiopathological processes and represent the target of about 30% of presently available drugs. After activation by an external ligand, they undergo a conformational change leading to the activation of one or several signaling pathways. Understanding the molecular mechanisms leading to GPCR activation and biased signaling (activation of a specific pathway) is an area of intense research to develop "biased" drugs with reduced side effects.

Using all-atom classical molecular dynamics simulations, we can observe activation-like transitions that occur on the millisecond timescale. We mainly focus on two receptor sets: (1) the chemokine receptors, involved in immune homeostasis and inflammation, and (2) the angiotensin II receptors AT1R and AT2R, involved in cardiovascular regulation.

Our study on the chemokine receptors (doi: 10.1371/journal.pcbi.1006209) reveals that the allosteric sodium binding site dramatically varies within this family. The dynamic simulations indicate that homeostatic receptors, such as CXCR4, have a very stable sodium binding site whereas inflammatory receptors, such as CCR5, have a loose site and an alternative, secondary binding site. Coupled to a phylogenetic analysis, these results suggest that this switch in the sodium binding mode played a key role in the functional evolution of chemokine receptors. They also reveal unanticipated roles of the sodium ion in the mechanisms of action of GPCRs. Better understanding of the sodium role will help improve drug design.
Study of Navier-Stokes 3D time discretization strategies on the efficiency of parallelization in PETSc

Université de Lyon, Institut Camille Jordan UMR5208-CNRS-U, Lyon1

DAMIEN TROMEUR-DERVOUT, UNIVERSITY PROFESSOR, SECTION 26

The objective of this project is to investigate a totally implicit temporal discretization of the Navier-Stokes equations incompressible in velocity-vorticity formulation leading, after spatial discretization of the six three-dimensional fields, to write a system of algebraic differential equations (ADE). The targeted test case is the problem of the lid driven cavity with a 3:1 ratio with a Reynolds number of 3200.

From a numerical point of view, this approach makes it possible to free oneself from the Courant-Friedrichs-Lewy condition limiting the time step compared to the space discretization step present in explicit or semi-implicit time discretization and allows control of the time step in an adaptive way by having a control on the error with the searched solution. Moreover, it does not introduce a time delay in the definition of boundary conditions on the vorticity, responsible for the formation of Taylor-Görtler vortex structures in the plane perpendicular to the flow. The choice of implementation with the PETSc open source library, makes it possible to have/develop powerful non-linear solvers to move from one time step to the next. In particular, Newtonian numerical techniques without the explicit construction of the Jacobian matrix (non-linear GMRES), make it possible to address significant computational domains for the complete cavity such as 768x256x256 points with six fields, thus an EDA system of about 302M unknowns with complex nonlinear dynamics.

Comparison of Taylor-Görtler structures for strategy 1 (respectively strategy 2) decoupled velocity-vorticity formulation with explicit time discretization (respectively semi-implicit) for the convection with the rest being implicitly discretized and for strategy 3 fully implicit time discretization velocity-vorticity, with 192x64x64 points and a dt time step = 0.005.
Pl@ntNet addresses the problem of the recognition of the world’s flora

ALEXIS JOLY, RESEARCHER AT INRIA

HERVÉ GOËAU, CIRAD, AMAP
PIERRE BONNET, CIRAD, AMAP
JEAN-CHRISTOPHE LOMBARDO, INRIA, LIRMM
JULIEN CHAMP, INRIA, LIRMM
ANTOINE AFFOUARD, INRIA, LIRMM / AMAP

Automated plant identification has improved considerably in recent years, particularly through advances in deep learning. In particular, several scientific studies have shown that it is now possible to obtain identification performances close to those of human experts. One of the most popular plant identification applications, Pl@ntNet, now operates on 25,000 plant species. This already makes it a very powerful tool for plant biodiversity inventorying, but it is still far from the 390,000 plant species currently known to science, not to mention the thousands of new species that are being discovered and described each year. One of the major challenges is therefore to match such systems to the scale of global biodiversity.

In an attempt to meet this challenge, the Pl@ntNet team, composed of researchers and engineers from four French research organizations, has created a reference image database of more than 11 million images of plants, illustrating nearly 296,000 species. Training a convolutional neural network on such a large data set on a standard machine equipped with four recent GPUs can take up to several months. In addition, to select the most efficient architecture and optimize hyper-parameters, it is often necessary to train dozens of networks of this type. Overall, this becomes a very intensive computing task that must be distributed over a large infrastructure.

The Pl@ntNet team used two of GENCI’s supercomputers, the Ouessant machine with 12 IBM Minsky nodes each with 4 Nvidia P100 GPUs, and the Irene machine, a BULL Sequana supercomputer with 1600 nodes each with 24 Intel Skylake nodes. The training time for a global flora recognition model was thus reduced to a few tens of hours, which enabled the Pl@ntNet team to obtain unprecedented results, with the hope of integrating these into the app in the near future.

The Pl@ntNet application developed by four French research organizations (Inria, CIRAD, INRA and IRD).

Geographic distribution of the images in the reference database used for the global flora recognition model learning.
Impact of GENCI for startups, SMEs and industry

Our actions with startups and SMEs

PRODUCTIVE COLLABORATION WITH FRENCH TECH CENTRAL

The Big Data, AI PARIS 2019 and RDV Carnot trade fairs were opportunities to build awareness in new companies and to present company projects through the use of workshops. These actions were supplemented with our presence at French Tech Central. Two workshops were held to present the service offers of GENCI and Inria aimed at SMEs. More than 60 companies attended these. More than 10 individual meetings were then held thanks to our presence every Thursday morning at Station F.

SIMSEO: A POSITIVE REPORT FOR THE 4TH YEAR

The fourth period of the SiMSEO, running from 1st October 2018 to 30th September 2019, made it possible to increase awareness within 353 new companies and to provide ongoing support for 22 of these. During the period, our main focus was on marketing actions working with an agency in order to best identify our target and thus undertake new targeting initiatives using the internet which will be rolled out in 2020. We have updated the SiMSEO web page to make it more relevant to its industry audience through, in particular, presentations of company Success Stories.
Our actions at the service of industrial competitiveness

GENCI: A CATALYST IN THE LINK BETWEEN PUBLIC AND PRIVATE SECTOR RESEARCH

Together with assistance for SMEs and startups through the SiMSEO project, GENCI’s computing and storage resources have also been made available to French industry for its open research projects (with the publication of the results). Thus, each year, of the 600 projects supported by GENCI, around 15% receive industrial support (public-private collaboration, CIFRE thesis, Chairs, etc.) highlighting the value of HPC and now of Artificial Intelligence, for industry in order to reduce design and maintenance times by means of digital twins, making their products safer or even more efficient in terms of resource use.

Among the many examples for 2019 there was the work by Safran and Renault (both linked with CERFACS) around the optimization of combustion in piston engines and in aero-engines, EDF with IMFT for multiphase simulation of fluidized bed reactors and l’Oréal (with Insitut Charles Sadron/CNRS) in the field of molecular modelling for cosmetics, and finally TheraPanacea, a promising startup in the field of Artificial Intelligence assisted medical imaging.
GENCI at the service...

p.43... of research and innovation
p.43... of users
Alongside the use of GENCI’s resources for academic and industrial research, 2019 was also a noteworthy year thanks to a major result in the field of technological innovation.

As part of the PPI4HPC project, GENCI chose the offer from ATOS for the upgrading of the Joliot-Curie supercomputer at TGCC with a new partition based around Manycore nodes (2 AMD Rome 64 core 2.6 GHz 280 W processors), with a direct water cooling system to more than 95% of its configuration. GENCI and ATOS were the first to present these technologies at the Top500 in November 2019, produced thanks to the work of CEA and ATOS teams. These were the fruits of an initial European R&D funding project (known as PCP) in which GENCI financed part of the cooling system, with the PPI4HPC project leading to the industrialization of these innovative solutions.

Beyond technical innovations, PPI is also a legal innovation. GENCI has been working with CEA (France), BSC (Spain), CINECA (Italy) and FZJ (Germany) on the operation of the European Public Procurement of Innovations for High Performance Computing (PPI4HPC) project covering the purchasing of computing resources for project members’ centers. GENCI, as the adjudication authority with responsibility for approving a cross-border competitive tendering procedure for the purchase of computer equipment with a matching contribution from the European Commission of up to 35% of the investment budget, finalized the Spanish and Italian procedures in 2019. The procedure will be fully approved in 2020 with the completion of the German procedure.

GENCI will then have fulfilled its role as the adjudication authority acting on behalf of all the various European actors.

At the same time as continuing monthly meetings with its users on the User Committees (COMUT) quarterly in the three centers enabling dialog on events and feedback on any new requirements among the users, GENCI has been out and about to meet its users and most particularly those working in the field of Artificial Intelligence in order to prepare for the launch of the Jean Zay supercomputer. Rennes, Paris, Saclay, Toulouse, Sophia-Antipolis, Grenoble, Bordeaux, Clermont-Ferrand, Lille: A real Tour de France to introduce the new features available on Jean Zay and gather details of the Artificial Intelligence requirements of the teams! This feedback was used in designing the environment for Jean Zay.
GENCI: Internal Organization

p.45 Latest on the Civil Society
p.46 Internal organization
p.47 Members of the Official Bodies
**Latest on the Civil Society**

The General Secretariat is a team of 4 people with responsibility for the organization’s administrative, financial, legal and human resources needs. It therefore deals with a wide range of matters, including most notably this year, the GDPR (General Data Protection Regulations), changes to the payment circuit and the setting up of a Social & Economic Committee.

**GDPR**

GENCI has been applying the provisions of the General Data Protection Regulations (GDPR) since their introduction in May 2018:
- Creation of the role of Data Protection Officer (DPO), assigned to our Legal Manager,
- Audit for the definition of the action plan,
- Initiatives to increase awareness among GENCI staff,
- Application of GDPR provisions to the eDARI process.

In 2019, GENCI continued its actions to ensure its compliance by reorganizing its personnel data and its Internal file server.

**DEMATIALIZATION OF THE PAYMENT CIRCUIT**

The invoicing and payment circuit has now been fully dematerialized with the installation of the software tools (financial management system, banking interface and accounting tools).

**HUMAN RESOURCES**

**Personnel changes within GENCI**

GENCI employed 15 people in 2019.

As full-time equivalent, the workforce is 13.23 with the following changes:
- 2 new people joined GENCI:
  - Christelle PIECHURSKI, as HPC Manager with responsibility for the Technology Watch Unit,
  - Marieke PODEVIN, as Legal Manager and DPO;
- Imène LITIM was a temporary Secretary who was recruited in her role,
- Over the same period, 2 people left the Company:
  - Laura PREUD'HOMME, Legal Manager,
  - Séverine SAINT HUBERT, Communications Manager.

**Internal Regulations and Charter**

In 2019, GENCI with the aim of formalizing its organization for its staff, confirmed:
- Its Internal Regulations,
- A remote homeworking Charter taking changes to the Company into account. The Charter allows remote homeworking one day a week.

**Election of representatives to the Comité Social Économique (CSE)**

Following on from the Macron Orders, the Social and Economic Committee (Comité d’Entreprise) and the Health, Safety and Working Conditions Committee (CHSCT) have been merged within the CSE. The requirement was that this body, with exclusive responsibility for social dialogue, was setup within all companies by 1st January 2020.

Given the size of the company, elections were held for an employee representative and an alternate employee representative for this body. Following a 1st round of elections without any candidates from the Trade Unions, the 2nd round of elections for personnel representatives was held on 17th December 2019. As a result, Mrs Elise Quentel was elected employee representative on the CSE. There was no candidate for Alternate Representative.

The first meeting of the newly constituted CSE was held on 28th January 2020.
Internal Organization in 2019

Management Committee

Philippe LAVOCAT
CEO

Edouard BRUNEL
General Secretary

Jean-Philippe PROUX
Operations and Security Officer

Stéphane REQUENA
Chief Technical Officer

Séverine SAINT-HUBERT
Communication Manager until 30/11/2019

Marie-Hélène VOUETTE
Partnership Manager

Administrative and Finance Department

Maïté CAMPEAS
Executive Assistant

Imène LITIM
Administrative Assistant
January to April and as of September 2019

Sandrine BASSIÈRES
May to September 2019

Laetitia PHO
Administration and Finance Manager

Marieke PODEVIN
Senior Legal Officer
Data Protection Officer as of 14/10/2019

Laura PREUDHOMME
until 28/02/2019

Technical and Operations Department

Christelle PIECHURSKI
HPC Manager with responsibility for the Technology Watch Unit

Elise QUENTEL
National Projects Manager: Equip@meso, SIMSEO

Philippe SEGERS
European Projects Manager

Delphine THEODOROU
Project Operations Manager

Communication

Annabel TRUONG
Communication Officer

GENCI | ANNUAL REPORT
MEMBERS OF THE OFFICIAL BODIES

As at 31/12/2019

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 GELLE - 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 Cynthia SAYEG. CEA representative: Mr Rémi KELLER. Inria representative: Mr François DAZELLE. 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. CEA representative: Mr Hervé CELESTIN, Head of Administration and Finances Service. CNRS representative: Mr Michel DAYDÉ, Scientific Delegate - Mr Denis VEYNANTE, Chairman of the Steering Committee of the Compute & Data Mission. Universities' representative: Mr Jean ROMAN, Deputy Scientific Director - Research Directorate for Applied Mathematics, Computing & Simulation - Mr Frédéric DESPREZ, Deputy Scientific Director for “Networks, Systems & Services”.

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 Denis GIROU, Director of IDRIS. CPU representative: Mr Francois BODIN, Professor @ University Rennes1 - Mr Boris DINTRANS, Director of CINES. Inria representative: Mr Jean Roman, Deputy Scientific Director - Research Directorate for Applied Mathematics, Computing & Simulation - Mr Jean-Frédéric GERBEAU.

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 Christian CHARDONNET, Head of the Department of Large Scale Research Infrastructures. 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.

GENCI would like to thank its Shareholders, Scientists, Center Directors and everyone else who has contributed to the writing of this Annual Report.

Publisher: Philippe LAVOCAT - Coordination: Annabel TRUONG - Design and Production: Backdrop - Printed by: Welcom Photos: © Cyril FREZILION/IDRIS/CNRS Picture Library, © CNRS Picture Library, © CEA, © CEA/Painting C215 © URCA, © AdobeStock, © French Tech Central, DR.

GENCI, 6bis, rue Auguste Vitu - 75015 Paris - France. Tél. : +33 (0)1 42 50 04 15 © GENCI - april 2020.