GENCI was created in 2007 by the government with the aim of placing France among the leading countries within Europe and on the international stage in terms of high performance computing. GENCI has five partners: The State, represented by the Ministry for Higher Education and Research, CEA, CNRS, French Universities, represented by the Conference of University Presidents (CPU), and Inria.

GENCI is actively working to **put in place an integrated high performance computing ecosystem**. At the national level, GENCI is responsible for implementing French government policy in the field of high performance computing in support of the scientific community. Around this objective, GENCI is coordinating the equipping of three national computing centres to create a combined computing peak power of just over 1.6 petaflop/s by the end of 2012, using different but complementary architectures. With the Equip@meso project, chosen in 2011 as part of the 1st “Equipements d’excellence” ("Excellence Equipment") call for the “Investissements d’avenir” ("Future Investments"), GENCI has extended this dynamic to the regional level, in association with ten university partners, covering all its components: hardware, training and links with industry. At the European level, GENCI represents France within the PRACE high performance computing infrastructure, of which it was a founding member. France is playing its full role within PRACE with the making available of the Curie supercomputer, designed by Bull and operated by the operational teams of the Très Grand Centre de Calcul du CEA (TGCC), in Bruyères-le-Châtel.

GENCI is also heavily involved in **promoting numerical simulation and high performance computing** within the French academic research world and with industry. This includes working with Inria and Oséo as part of a specific initiative aimed at the SME sector. Conducted in partnership with five competitiveness clusters, this initiative supports SMEs in assessing the productivity and competitiveness gains that can be achieved through the use of high performance computing.

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It has been an exciting five-year period during which France has been able to resume its place among the leading nations in the field of high performance computing. This success story was initiated by our partners: the Ministry for Higher Education and Research, the CEA, the CNRS, the Conference of University Presidents and Inria. Without their ongoing commitment and support from 2007 onwards, we would not have been able to achieve what we have today.

This collective endeavour has benefited users of high performance computing in both the fields of scientific and industrial research, drawing in particular on the skills of the teams at the three national computing centres –the CEA’s Très Grand Centre de Calcul, CNRS’s IDRIS and CINES for higher education. The role of GENCI has been to act as the link between all the high performance computing players in France and to facilitate, whenever possible, access to these high performance resources.

Five years ago it was a gamble. Today more than 600 projects a year are hosted using our national resources and a number of world firsts have been achieved across all disciplines, as can be seen both in the report from the Chairs of the ten GENCI Subject Panels (see page 11) and the ten results we have chosen to highlight (see page 15). These are simply a few examples of the advances achieved in 2012 using the national computing resources but they are perfect illustrations of the science that supercomputers make possible.

Following Jade at the CINES in 2008, Titane and Curie at the TGCC in 2009 and 2011, GENCI has continued its work to enhance France’s national computing assets, with the installation of the Ada and Turing computers at the IDRIS in 2012, taking the power now available to French researchers to just over 1.6 petaflop/s peak.

As the report on the 2012 Campaign (see page 6) shows, GENCI’s resources have been used to their maximum potential and demand remains ahead of supply, a sign of the attractiveness of the computing resources.

This level of vigour has also been made possible by the commitment of the teams of the three national computing centres (see page 8) who ensure the day-to-day operational availability of the equipment, as well as providing assistance to users.

Other equally important results were achieved in 2012. At the European level, the French scientific and industrial communities were among the leading beneficiaries of the computing time allocated by the PRACE European high performance computing infrastructure (www.prace-ri.eu) of which we were both founder members and one of the funders with the making available of the Curie supercomputer.

Thanks to the Equip@meso project, coordinated by GENCI and involving ten universities and academic partners, regional computing resources have been significantly increased, in harmony with the stated objectives, from 500 to 780 teraflop/s in just two years.

Some thirty small companies, working in all fields, are currently receiving support from under the HPC-PME (HPC-SME) Initiative, launched by us two years ago together with Inria and Oséo and aimed at helping SMEs wishing to integrate high performance computing into their growth model. We remain totally committed to achieving our objective: To make high performance computing a state-of-the-art tool of the production of knowledge and innovation.
“The impact of high performance computing is set to grow”

A foreword by Olivier Pironneau, Chair of the GENCI Evaluation Committee

Report on the year ended

At the international level the power of supercomputers continues to increase, with the scientific need and demand for it growing at the same time. In Europe, PRACE has now reached a level of maturity and that is good news.

In France then, although we now have just over 1.6 petaflop/s on a variety of architectures, we have already reached a critical level of saturation. The demand for computer hours on the GENCI resources continues to grow strongly and it only takes one machine to be out of operation for a short time for there to be serious repercussions. We are truly operating at “just-in-time”!

I have also noted that the number of researchers making use of high performance computing has changed little but high performance computing has become more central across all disciplines. By way of evidence I would refer to the results achieved in astrophysics in 2012, the simulation of the evolution of the structuring of the whole of the observable Universe, which was really spectacular... There is also the outstanding work in climatology for the production of the 5th IPCC Report, which required a great deal of computing time and an ad hoc organisation to achieve the defined objectives. Another project is the Human Brain Project which is a huge challenge and is now supported by Europe.

2012 was also a year of technical advances. In the field of programing methods, first of all, progress was made in increasing the portability of applications on hybrid machines. This was an excellent result that should help facilitate and extend the use of these machines.

There is also the matter of electricity consumption, an increasingly critical element to take into account. A number of advances have been made with low electricity consumption processors, on cooling, and the European Mont Blanc project has produced some interesting results... The ball is however very much in the equipment manufacturers’ court!
Finally, the issue of processing what is known as “big data” remains alive and unresolved.

In terms of training, the situation has changed little... Despite the mesocentres, together with centres such as Cerfacs and entities such as the CNRS Groupe Calcul (computing group), working well to provide short training courses, there is still not enough training in high performance computing, even within the scientific disciplines themselves, for their Masters and Doctoral students.

There are other elements that need to be taken into account. First of all the work of the ANR, which I want to acknowledge, which has now added high performance computing to its priorities; next there is the publication by the CNRS of a White Paper mapping the use of high performance computing across all disciplinary fields and that lists almost 2,500 researchers and teaching-researchers involved. That is a very big community, one of the largest in Europe.

More generally, the impact of high performance computing is set to grow, whether in terms of scientific advances such as those covered in this report, its use within advanced industrial practice (aeronautics, automobile, energy, etc.), or its spread to the SME sector, notably through the initiative supported by GENCI, Inria and Oséo.

The outlook

The turning point, naturally, will be computing using millions of cores, at the exascale due to be achieved as forecast before 2020 but prior to that we need to make sure the researchers are ready for this level of power and making use of the full potential it offers... I can see two possible inhibitors on the take up of exascale by researchers: Firstly, with scientific applications that are too difficult to implement - there is a lot of development work, and it is donkey work, still to do in this field; secondly, the lack of technical training.

The changes of the last five years

The structure that has been created by GENCI since 2007 is bearing its fruit. High performance computing has been “resuscitated” and France now has an effective national policy for high performance computing. The objectives that were set have clearly been achieved! High performance computing is thus doing pretty well in our nation even though the equilibrium of the ecosystem has not yet been completely established.

2012 was the year of the power build-up in the regional computing centres, partners in the Equip@meso project... We need to continue along this path.

Image of brain development, measured by nuclear magnetic resonance (NMR): Work led by a French INSERM/CEA team, as part of the Human Brain Project © INSERM-CEA
Heavy Call on National Computing Resources

As in previous years, GENCI’s resources, with an average annual load of almost 80%, were used at maximum capacity in 2012. The number of projects submitted remains stable whilst the average number of hours requested per project increased. In global terms, the number of hours requested in 2012 on the main computers was 1.4 times greater than the number of available hours. The scientific projects are mostly being carried out by mixed teams.

A total of 535 million hours allocated... That was the remarkable achievement of GENCI in 2012 with the opening of the so-called “nœuds hybrides” (“hybrid nodes”) and “nœuds fins” (“thin nodes”) of the Curie supercomputer, following the “nœuds larges” (“fat nodes”) phase the previous year, which had increased the number of computing hours available to the French scientific community.

During the two sessions of the 2012 Campaign, organised respectively in September and April for the January 1\textsuperscript{st} and July 1\textsuperscript{st} allocations (see box), of the 622 projects submitted, 600 were granted (615 in 2011), over a quarter of which were new projects (27% compared with 23% in 2011).

There was a similar stability for the distribution of projects by the Subject Panels (Comités Thématiques - CT). All scientific communities were able to benefit from the country’s computing resources, with a multi-disciplinary use.

As a symbol of the attractiveness of the computing resources, the rate of demand was, as an average, 1.4 for all the machines. And despite an additional 60 million hours being made available thanks to the thin nodes phase at Curie, as in 2011, total demand remained well ahead of the supply.

Access to the national computing resources is based on a project call process, implemented twice a year by GENCI. Scientists, from eligible organisations (mainly public sector research), submit requests for computing hours with a statement of the hoped for results. These requests are evaluated by GENCI Subject Panels (Comités Thématiques - CT) which cover all scientific disciplines.

The actual rate of consumption was also sometimes greater than the theoretically allocated computing hours, evidence of the very good availability of the equipment thanks to the teams at the national computing centres.

Hours granted by GENCI in 2012, were on the Titane and Titane GPU computers, the Curie fat nodes, Curie thin nodes and Curie hybrid nodes at the TGCC, the Babel and Vargas computers at the IDRIS, the Jade and Yoda computers at the CINES.
Taking all the centres together, the project submitters benefited from an allocation of computing hours concentrated mainly in seven regions (see opposite): Ile-de-France (157 Mh), Provence-Alpes-Côte d’Azur (102.6 Mh), Rhône-Alpes (58.7 Mh), Haute-Normandie (52.9 Mh), Midi-Pyrénées (34 Mh), Aquitaine (26.2 Mh) and Nord-Pas-de-Calais (21.3 Mh).

The numbers of projects requesting over a million hours has been increasing year-on-year: 44 projects in 2010, 80 in 2011 and 88 in 2012. These projects were granted on the Curie thin nodes (TGCC, 20 projects), Titane (CCRT, 14 projects), Babel (IDRIS, 23 projects) and Jade (31 projects). All themes were covered with, however, a predominance for CT2 (fluid mechanics, reactive fluids, complex fluids), as well as CT4 (astrophysics and geophysics) and CT5 (theoretical physics and plasma physics).

233 projects were supported by the French National Research Agency (Agence Nationale de la Recherche - ANR), representing 38% of projects. This was a slight decrease on 2011 (42%) coinciding with the end of the three-year period for certain projects.

88 projects (82 in 2011) reported receipt of industrial support (collaboration with a research laboratory), representing 14% of projects. These projects were mainly from CT2 (fluid mechanics, reactive fluids, complex fluids) with 36 projects (41%) and CT9 (physics, chemistry, material properties) with 18 projects (20%).

As in 2011, a majority of the work (57%) made use of fewer than 256 cores. The proportion of those using more than 1,024 cores however was up significantly (11% in 2012 compared with 7% in 2011). This opened the way for the use, in the short-term, of the Tier0 computing resources contributed by the PRACE research infrastructure. Projects using 256 to 1,024 cores (25%, identical to 2011) represent a significant pool of applications that could in the medium-term also migrate to Tier0 resources.

With an annual average load of almost 80%, GENCI’s resources are being used at their maximum. The introduction of Curie in 2012 and the renewal of the computers at IDRIS should help in 2013 to achieve a total capacity that better matches with the continued high level of demand.

At the end of 2011, GENCI surveyed the users of the national computing resources in order to draw up an initial report on the last five years. This survey, relatively fruitful, (22% rate of response), revealed a level of overall satisfaction as well as a feeling that there was a lack of information on the ecosystem and accessible resources.
With responsibility for making priority investments in the field of high performance computing for French academic research, GENCI acts as the contracting authority for the national computing resources, spread across three centres: the Très Grand Centre de Calcul du CEA (TGCC), in Bruyères-le-Châtel, the Institut du Développement et des Ressources en Informatique Scientifique (IDRIS) at the CNRS, in Orsay, and the Centre Informatique National pour l’Enseignement Supérieur (CINES), in Montpellier. These three computing centres carry out the project management roles for the equipment.

Christine Ménaché, CCRT Project Manager, Denis Girou, Director of IDRIS, and Francis Daumas, Director of CINES, look back on 2012.

Christine Ménaché, CCRT Project Manager

At the TGCC, 2012 was, above all, a year in which Curie reached full power. Access to the Curie thin nodes for the realisation of the “Grands Challenges” at the very beginning of 2012, well ahead of schedule for production, called for a great deal of work by the CEA’s teams over a number of months prior to the complete opening of the supercomputer, on 1st March 2012, with very close supervision of the first users.

At the same time, the CEA application support managers for the TGCC were also involved in the technical expertise of the projects submitted as part both of the PRACE Preparatory Access Calls, and the Regular Access Calls.

Alongside this the CEA’s teams were active in the implementation of the PATC (PRACE Advanced Training Centre) France, supported by the Maison de la Simulation, with the aim of offering PRACE users advanced training in the optimised use of the Curie supercomputer and its environment.

Finally, 2012 was the year in which Mercure came to an end, on completion of the CMIP5 (Coupled Model Intercomparison Project Phase 5) Campaign. The flood of data generated by that campaign highlighted the need for greater anticipation and increased collaboration between user communities and the computing centres on these data management themes that are now one of the key elements for HPC. As a result regular meetings have been instituted with the aim of ensuring the longevity of the results of the CMIP5 campaign and preparing for the next IPCC (Intergovernmental Panel on Climate Change) campaigns.

Denis Girou, Director of IDRIS

At IDRIS, the main event in 2012 was essentially that of the replacement of the former supercomputers, installed in 2008. Following a tender call launched by GENCI in autumn 2011, the choice was for two supercomputers with complementary architectures, from IBM, with a total nominal peak performance of 1 PFlop/s.

One of these, called Turing in honour of Alan Turing (1912-1954), is a Blue Gene/Q massive parallelism type with more than 65,000 cores and 65 terabytes of main memory. The other one, called Ada after Ada Lovelace (1815-1852), has 332 nodes x 3750, a huge memory and Intel Sandy Bridge processors, with more than 10,000 cores and 46 terabytes of main memory.
There are an additional four pre- and post-processing nodes, each with 32 cores and a very large shared memory of 1 Terabyte, with the configuration including a 2.2 Petabyte shared file system. This new configuration was installed in the second-half of 2012 and was open for all our users as of 01 January 2013.

As is normal practice in the acceptance phase for new supercomputers, these were opened subject to specific conditions to a number of projects for the performance of thirteen “Grands Challenges” on the two computers, making possible significant advances in several research fields.

Francis Daumas, Director of CINES

The CINES in 2012, bearing in mind the future challenges, focussed on its preparations of the new infrastructures and the implementation of a new data architecture.

Over the year, the scale drawings for a new 600 m² machine room, equipped for “warm” water-cooled machines, were produced, the project manager and the contractors selected. Delivery is scheduled for the second-half of 2013.

At the same time, a dedicated 10 MW ERDF line was added to the existing 2.5 MW line, ensuring that CINES has the power capacity to meet upcoming needs and helping to enhance the overall reliability of the infrastructures.

A new data architecture has been defined and implemented at the beginning of 2013: This is based on a design known as “datacentric”, placing the data at the centre of the organisation by means of a shared Lustre space and the implementation of PDMF (Parallel DMF).

The PRACE prototypes, notably “Exascale I/O”, have been the subject of fruitful collaborations with two other national centres.

In the context of its involvement in PATC France, the CINES carried out initial training on visualisation, in November 2012.

Finally, in terms of the second mission of the CINES, the long-term preservation of digital data, new projects, including some relating to very large volumes of data, saw the light of day (with Inserm, IRHT, University of Lorraine, etc.), alongside the operational aspects of the digital archives.

At the same time, CINES was involved in the implementation of the European collaborative data infrastructure, supported by the Eudat European project.
Two project access calls are held every year for all users (academic or industrial) wishing to access the national computing resources for work that is being carried out in a public research or higher educational body.

The first project access call is held in the final quarter of the year n-1 for the allocation of hours as of 01 January of year n; this covers the submission of new projects or the renewal of current projects.

The second, supplementary, project access call is held during the second quarter of the year n for an allocation as of 01 July of the same year; this covers the submission of new files or supplementary requests for files accepted for the first session.

Applications are submitted to the website: www.edari.fr

The selection is made on the basis of the scientific excellence of the research project, with an obligation to publish the results.

To encourage users to make planned use of the allocated resources, there is an adjustment procedure at the end of the first three months of the year n. The application of this adjustment procedure may lead to a withdrawal of up to 40% of the time initially allocated.

In addition, throughout the year, supplementary hours can be granted to current projects as exceptional measures; these “as needed” requests are submitted through the DARI portal.

The ten GENCI Subject Panels (comités thématiques - CT)

CT1: Environment
CT2: Fluid Mechanics, Reactive Fluids, Complex Fluids
CT3: Biomedical Simulation and Health Care Application
CT4: Astrophysics and Geophysics
CT5: Theoretical Physics and Plasma Physics
CT6: Computer Science, Algorithms and Mathematics
CT7: Organised Molecular Systems and Biology
CT8: Quantum Chemistry and Molecular Modelling
CT9: Physics, Chemistry and Material Properties
CT10: Multi-disciplinary Applications and New HPC Applications
Increasingly Realistic Simulations

The Chairs of GENCI’s ten Subject Panels report on 2012 for their respective fields and outline what is in prospect for the coming years. As in previous years, they are all keen to highlight the quality of the projects submitted to them as well as the results obtained, getting ever closer to the reality of the phenomena in question. In the space of five years, with the significant increase in national resources, French researchers have extended the scope of their investigations and made advances in the accuracy of their models.

2012 Report and Outlook for 2013

Patrick Mascart, Chair of CT1 (environment)
The projects we selected, just about the same number as in 2011, are mostly planned to continue over several years, which is what one would expect for the development of software relating to climate, oceanography and environmental modelling: 4 projects are new projects, 51 are multi-year projects. These resulted, in 2012, in around a hundred publications in leading international peer-reviewed journals.

As was announced last year, the allocations to CT1 in 2012 made it possible to produce climate simulations for the IPCC (Intergovernmental Panel on Climate Change). The delivery of these simulations saw the start of the final phase of analysis and interpretation of the results, which will lead to the issuing of the final report of the IPCC in 2013.

A major achievement, the bringing online of the Curie supercomputer at the TGCC made it possible, for the environment as well as for oceanography, to start the work on the large computational grids and opened the way towards high resolution spatial simulations.

Luc Vervisch, Chair of CT2 (fluids mechanics, reactive fluids, complex fluids)
There has been a strong increase in the quality of the scientific dossiers, in many cases with a direct link between the GENCI allocation of time, and support for the project by the Agence Nationale de la Recherche (ANR) or the European Research Council (ERC). There has been a quasi-exponential growth in the number of simulations using tens of thousands of processors, which is a confirmation of the serious commitment within the ‘fluid mechanics’ community to high performance computing. This can be seen in terms of the increasing number of publications in the leading scientific fluid mechanics journals.

Marc Thiriet, Chair of CT3 (biomedical simulation and health care application)
The tools developed in the field of biology and health are based on a multidisciplinary approach. The modelling and the numerical simulation of complex phenomena make use of coupling platforms (chemical reaction cascade, electrophysiology, continuum mechanics, mass and heat transfers, etc.). High performance computing therefore has a real contribution to make but the lack of perfectly adapted tools is slowing its development.

Édouard Audit, Chair of CT4 (astrophysics and geophysics)
There has been a 10% increase, compared with 2011, in projects relating to our themes. This increase is entirely down to astrophysics with 40 projects, with geophysics unchanged and 15 projects. The rate of renewal has also remained relatively stable for a number of years, at around 25 to 30% of new projects, each year.

Of these new projects, a significant proportion are projects re-emerging after one or more years of absence on the national resources. The number of projects receiving financial support has been growing for several years.

In 2012, 24 projects were supported by the ANR, 16 received European funding (ERC, etc.), and 16 received funding from other sources (national, regional programmes, industrial contracts, etc.). More than 20% of projects had multiple funding sources.
Sylvie Jacquemot, Chair of CT5 (theoretical physics and plasma physics)

Our themes cover a wide range of distinct subjects in which digital modelling has a key role. This thus covers issues in plasma physics (fundamental and applied, for magnetic fusion or inertial fusion), particle physics (including network QCD) and nuclear physics, electromagnetism and theoretical physics, notably the study of the electronic properties of solids and condensed matter.

The quality of the proposals, up 26.3% compared with last year, continues to be excellent. Twenty-three articles were published in 2012 in peer-reviewed journals, mainly relating to plasma physics (eight articles) and electromagnetism (seven).

Most of these were from projects submitted in previous years (28.3% in 2010 and 47.8% in 2011).

Jacques Blum, Chair of CT6 (computer science, algorithms and mathematics)

The submissions in 2012 were of a very high level and were more or less equally split between two categories.

First, those relating to parallel computing algorithms in all forms: resolution of large sparse linear systems, preconditioners, grid generation, eigenvalue methods, optimization algorithms, parallel programming languages...

And second, those more specifically dedicated to digital algorithms: evolutionary algorithms, optimization and control, finite elements method, particle methods, domain decomposition, multi-grid methods...

From all of this work, in 2012, there were at least 30 publications in peer-reviewed journals or reviewed international conference proceedings.

The outlook looks very promising: Exascale algorithms are set for rapid expansion to ensure that digital resolution methods are in a position to make the most of the performance potential of future computers.

There is still a great deal of work needed both in parallel computing science (communication between processors, etc.) and in digital algorithmics (large linear system, meshing, etc.).

In each of the application themes, we will be working to optimise the algorithms on the basis of the computers being used.

Yves-Henri Sanejouand, Chair of CT7 (organised molecular systems and biology)

In the majority of cases within our themes, these are ‘simple’ simulations of the molecular dynamic of large systems of biological interest (notably membranous proteins). These simulations are, however, increasingly playing a part in completing or enabling the interpretation of experimental data obtained through biophysical approaches (X-ray crystallography, NMR, fast AFM, etc.). This is undoubtedly because the microsecond scale is accessible and that at this timescale, many phenomena associated with the function of biological macromolecules can now be observed.

Marie-Bernadette Lepetit, Chair of CT8 (quantum chemistry and molecular modelling)

The proposals submitted were for the most part of good quality and the proposed research themes always extremely vast: very sophisticated computing on the spectroscopy of small systems (for astrophysics, among others) using sophisticated techniques for processing the electronic correlation, computing the structure or reactivity for very large molecules, nanosystems and solid phases, computing quantum dynamics and thermodynamic properties, etc.

There were, in 2012, 406 publications in peer-reviewed journals.

Alain Pasturel, Chair of CT9 (physics, chemistry and material properties)

A feature of 2012 was the scale of the increase in requests for computing time, in particular on the massively parallel and hybrid architectures. 80% of projects are of excellent quality, with an outstanding level of publication: an average of 3 to 4 publications per project in leading scientific journals.

Also in 2012, there were more new projects (around twenty), marking, in most cases, the arrival of young researchers, which is another indicator of the tremendous vitality within the community. The fields of application continue to deal with major issues facing society, such as energy (nuclear and renewable), the environment, health and also nanotechnologies.

The outlook is one in which continuity plays a major role.

In terms of ab initio type simulations, we are moving towards ever more precise computing and an ever wider spectrum of properties. These simulations are...
now a fundamental tool, increasingly forming the interface between a model theory and an ever-more complex experimental reality. The emergence of projects making use of multi-scale simulations is going require the ability to perform realistic simulations that make it possible to integrate different time and space scales.

**The changes over the five years**

*Patrick Mascart (CT1):* Over the five years, climate, ocean and atmosphere science projects have really benefited from the increase in high performance computing capacities delivered by GENCI. Progress has been made both in scientific and technological terms, and this has undoubtedly benefited climate modelling in particular.

Just five years ago, global climatic and environmental simulations were performed entirely using vectorial computers with a very small number of processors (a few units) and French work in the field was lagging significantly behind that being carried out in some other countries. Now we can access global climatic simulations. The improvements in the parallel computing capacities achieved by GENCI have been decisive because it has created a dynamic toward the future.

A second decisive advance made possible by the increase in computing capacities relates to the simulation of all atmospheric and oceanic flows. Here again, a matter of years ago, the need to use the whole amount of power available to achieve an acceptable computing resolution meant that only a very limited number of simulations could be performed. It is now relatively easy to obtain a satisfactory resolution, and the simulations are performed in groups of tens. This so-called “ensemble simulations” approach makes it possible to quantify the quality of the results by calculating the probabilities. This progress has been decisive because it means that the environmental disciplines have been able to adopt a much more rigorous and quantifiable methodology in the follow-up of the results.

Finally, the increase in the computing capacities achieved by GENCI has also made it possible to profoundly improve the taking into account of observation data in the modelling of natural phenomena, by generalising the variational assimilation methods. Five years ago, the extremely high cost of these techniques restricted their use to a few fields such as operational meteorological forecasting, and for classical data such as occasional in-situ observations. Now, these methods are standard for most geophysics disciplines, from environmental sciences, and oceanography to biogeochemical processes. In addition, the range of observations that can be assimilated has been hugely extended, for example as far as the assimilation of remote satellite or radar detected observations in the atmospheric sciences.

*Luc Vervisch (CT2):* The most noteworthy point of the last five years has undoubtedly been the use of high performance computing for the detailed analysis of flows, no longer just for simplified academic geometries but also for the realistic situations for systems encountered by the industrial partners of CT2 teams. This has opened new perspectives for the development of advanced analytical and design methods, based directly on the information obtained through high performance computing.

*Marc Thiriet (CT3):* There has not been a huge variation in the themes over recent year. Although a number of projects in the fields of nanotechnology and agronomic research fields have not been subject to renewal requests, we have seen the advent of new proposals relating to cellular signalling networks and anti-cancer treatments.

*Édouard Audit (CT4):* In recent years, a number of teams have made significant steps towards the massive parallelisation of their codes. Although there have not been any major thematic evolutions, the increase in national computing resources has enabled an increase in the spatial and temporal resolution of
the issues covered and the performance of simulations with more realistic models. Parametric studies on systems with very large number of degrees of freedom are also now possible. Among the scientific results obtained in recent years, I would highlight the performance of the first simulation of the evolution of the structuring of the whole of observable Universe, which is still a record achievement, the creation of a large catalogue of galaxy collisions that is useful both as a theoretical tool and for detailed comparisons with observations, significant progress in the dynamic of the interstellar milieu and the formation of stars, as well as on the dynamic and formation of planetary systems. In terms of geophysics, important progress has been made in the analysis of earthquakes and tsunamis, as well as in the methods of imaging and the reconstruction of subsoils. All of these results have extremely important repercussions for society as a whole.

Sylvie Jacquemot (CT5): The number of proposals submitted to CT5 since 2009 has remained relatively constant whilst the volume of hours requested has fluctuated over the years. The numerical tools, community-based for some, are subject to constant adaptation. At the same time, the community is growing, with new users who, following the validation of their numerical tools on local computers (possibly the mesocentres), bring these to GENCI’s resources for parametric studies. The older users, in turn, are beginning to make highly effective use of the resources of PRACE for their “flagship” applications. Some themes are positively flourishing, as a result of the level of maturity reached with the numerical tools, and the possibility of performing scale 1 simulations, with an ever-increasing social impact and above all, specifically in plasma physics, the fundamental requirement for dimensioning future experiments on major national and European research instruments currently under construction.

Jacques Blum (CT6): The projects do not, generally, require huge amounts of time but they do require resources on several machines to compare the performances of algorithms and libraries developed on the basis of the available parallelism structures. The diversity of the resources made available to the national community by GENCI is very important, enabling numerical experiments using several machines and for a limited number of hours on each of them.

The development and validation of methods is in essence the specificity of the work performed in the context of CT6, much more that the use of the codes for a dedicated application.

Yves-Henri Sanejouand (CT7): The timescales that are of real interest in terms of molecular modelling are those typically taken by a molecule of therapeutic interest to reach its binding site or for two proteins to “recognise” each other, and are, in most cases, two or three orders of magnitude beyond the microsecond. Work on the sub-millisecond scale has been going on across the Atlantic since 2012, with specialised supercomputers. Simulations at this scale enable notably a direct confrontation with much more plentiful and often much more detailed experimental data (notable structural), which are already helping to improve the models used.

Marie-Bernadette Lepetit (CT8): In recent years there has been a much greater level of interaction with experimenters: computing is today used much more as a way of helping to understand the experimental results, but with, more recently, an increase in the use of computing to explore the field of the possible prior to the manipulations. Another trend has been an increasingly multi-disciplinary approach. More and more proposals are now at the interface with solid physics, molecular physics, geophysics and biology. Finally, the use of massively parallel computers is rapidly increasing.

Alain Pasturel (CT9): Over the last five years, numerical simulations based on ab initio computing have increased significantly. These form over 80% of CT9 projects and have become a key support in the interpretation of the properties of most materials and in the development of new technologies. A lot of work has gone into the parallelisation of these computing codes to make use of the hundreds of computing cores and, in the last two years, the switch to massively parallel and hybrid architectures has become a reality.

Thierry Massard (CT10): By carrying out “educational” work around CT10, we should be able to attract a larger number of proposals in themes combining science and engineering. There will also a significant growth in the multi-disciplinary fields because HPC will make it possible to tackle highly complex topics. It will be a real challenge in the years to come.
First in the Fight against Forest Fires

the Latest in the Stars

Materials under surveillance

More Realistic Climate

Small Doses, Great Accuracy

Tracking Nerve Pulses

In the Wake of Lasers

Improving Control of Fusion

More Refined Model

Boosting Solar Energy
EVERY YEAR, thousands of hectares of forest in southern France, and especially in Corsica, go up in smoke, causing serious environmental, and sometimes human, damage. How does a fire get going and then spread? What are the factors that speed it up or slow it down? What are the environmental impacts?

Fire simulators are already used to provide operational assistance for firefighters in estimating how a fire progresses. But it was a world first developed by a team at the Sciences Pour l’Environnement (Environmental Sciences, SPE) Laboratory, a joint CNRS/University of Corsica team: To couple its fire simulator with the Meso-NH meteorological model (developed by the Laboratoire d’Aérologie (Aerology Laboratory) in Toulouse and Météo-France CNRM (French Meteorological Service – National Meteorological Research Centre) to examine fire phenomena on all scales, from the very smallest (submetric) to the largest (kilometric), from the dynamic of the flames and including the impact of the fire on air quality and the atmosphere in general, as well as the phenomena occurring in and around the fire. The project received funding from the ANR and received support from a number of partners (Cerfacs, Inria, M2P2, and EM2C).

For the study model, the researchers chose a fire that, during the summer of 2009, destroyed more than 3,000 hectares of forest around the village of Aullene in Southern Corsica. “By simulating the first 10 hours of the propagation of the fire, covering 2,000 hectares, we made a major step forward in the study of the fire-atmosphere feedback”, Frédéric Bosseur, Research Engineer and responsible for the parameterisation for the test case in the project, explained. Because, with this simulation, the phenomena occurring within the fire could be described with a remarkable degree of precision: The rise in the temperature of vegetation, generation then full fire of gas, advance of the fire front under the effect of the local topography, etc. The researcher explained, “This simulation also made it possible to refine our understanding of the impact of the fire very locally, namely local winds created by the intense heat of the fire and which then in turn modify the behaviour of the fire front”. Essential is the knowledge in estimating as accurately as possible the composition and movement of the smoke plumes as well as the release of pollutants into the atmosphere.

“In order to include the whole spectrum of the fire, this novel multi-disciplinary approach required a huge amount of computing resources”, Frédéric Bosseur pointed out. The simulation of other large fires, namely with a detailed description of the atmospheric chemistry and the comparison of the results with experimental data, is the next challenge for the research team.

The flame propagation codes, developed as part of this project, have been made available to the scientific community. These enabled the simulation of the advance of the lava flow and the smoke plume observed during the eruption of Piton de la Fournaise, on Reunion Island in 2007, in collaboration with the Laboratoire de l’Atmosphère et des Cyclones (Atmosphere and Cyclone Laboratory), a CNRS/University of Réunion/Météo France unit.

Modelling Forest Fires (CT2)
Principal Investigator: Jean-Baptiste FILIPPI, Environmental Science Laboratory (SPE)
GENCI Resources: Jade (CINES)
Increasing the yield from renewable energy sources is a vital challenge for society. The photovoltaic cell, the purpose of which is to capture the energy of sunlight, is currently the subject of intense research. Most of the photovoltaic panels currently installed use silicon, but the cost of the ultra-pure semi-conductors used in their production is a factor holding back even wider spread use of the technology.

A new option has been identified in making the most of this stupendous energy supply: hybrid photovoltaic cells, also known as dye-sensitized solar cells.

The idea is to use a dye which, under the effect of light, acquires enough energy to very rapidly inject an electron into a nearby semi-conductor. This process makes it possible to separately optimise the phenomena of the absorption of the light (by the dye) and the transport of the electrons (by the semi-conductor). However, with the addition of a solvent and the necessary additives the system becomes too big and too complex to be analysed in detail using the numerical tools specific to theoretical chemistry on conventional computing resources.

Carlo Adamo and his team at Chimie Paris-Tech were able to simulate, at a quantum level, the electronic interactions of several hundred atoms, on the Turing supercomputer installed at IDRIS and using the massively parallel CRYSTAL code, developed at the University of Turin.

In a day, thanks to the parallel use of several thousand computing cores, the researchers performed some ten optimisation cycles for the structure of the photovoltaic cell components (semi-conductor, dyes, additives and solvent) and were able to estimate the future energy yield using a computing protocol developed within the team.

The protocol, tested on known systems, was applied to new systems in the course of the project. By thus analysing the properties of tens of different molecules, Carlo Adamo and his team were able to quickly focus on a number of promising candidates, to the stage of testing, under real conditions, one of these dyes. The most promising molecules were then synthesised, and the experimental measures confirmed the theoretical predictions. These 2012 results were published in the Journal of Physical Chemistry Letters in 2013.

Although the efficiency of these new photovoltaic cells is, for the time being, poorer than that of conventional silicon cells, they do have the advantage of being cheaper, flexible and semi-transparent.

Grounds therefore for believing there will be new uses, and even more intense research in this field.

Modelling Hybrid Photovoltaic Cells (CT8)
Principal Investigator: Carlo ADAMO, Chimie Paris-Tech
GENCI Resources: Turing (CNRS/IDRIS)
Visualising the activity of cells in order to detect anomalies or even pathologies such as cancers... That is what Positron Emission Tomography (PET) makes possible. This method of medical imaging involves the injection of a molecule tagged with a short-life (maximum of a few hours) radioactive atom (carbon, fluorine, nitrogen, oxygen, etc.) and then observing its gradual disintegration, in positrons and then in photons. The detection of photons makes it possible to pinpoint the site of emission, and to reconstitute the tracer concentration in three dimensions (3D) at each point of the targeted organ.

How can this exploration be improved at the same time as reducing the doses introduced into the patients? This is real challenge for public health for increasing the well-being of both patients and healthcare staff as well as for extending the use of a system that has proven its effectiveness in oncology and neurology to other clinical fields, for instance pediatrics. That was the objective for the project working for the last four years with a team from the Modelling, Simulation and System Laboratory (Laboratoire de Modélisation, Simulation et Systèmes, LM2S) at the CEA Technological Research Division, DOSEO platform (Direction de la recherche technologique, plateforme DOSEO), in collaboration with Claude Comtat of the Frédéric Joliot Hospital Service (Service Hospitalier Frédéric Joliot) at the CEA Life Sciences Division (Direction des sciences du vivant du CEA).

“We developed an algorithm that allowed the reconstruction of the entire distribution of the tracer both in space and in time, in 4 dimensions, based on the data obtained by the PET and with an arbitrarily fine step”, Eric Barat and Thierry Montagu, researchers at LM2S explained. The originality of the project? It allows the reconstruction of the events detected by the PET sensors in the form of a space-time continuum and not as the normal juxtaposition of discrete functions (of “usual” images consisting of voxels, volumetric elements or 3D pixels). The method (known as Bayesian) supplies, among others, the uncertainty associated with any point in space (3D) and time (4D), which is why we talk of quantitative PET imaging. “Initially”, the researchers explained, “we had validated this novel approach with ‘virtual’ data. By repeating the calculations a very large number of times to get a good statistical series, we proved that our method made it possible to reconstruct the distribution with a reliable uncertainty”. The switch to real data turned out to be just as remarkable: “Once again, with lower doses, we obtained reconstructions of an equivalent quality to those obtained with the doses normally given to the patients”.

There is naturally a cost to all this work... in computing time. “The laboratory’s small cluster enabled us to develop the algorithm, but we needed more computing power to process the huge volumes of data”, Eric Barat pointed out. “Typically”, Thierry Montagu added, “a 4D reconstruction takes 24 hours using 1,000 computer cores”. The next stage: using the computing power of Curie to “prove that with a dose comparable to clinical doses, the results obtained are identical”.

With this aim in mind, the team has been allocated Preparatory Access, in 2013, to test the scalability of its code. But that is almost another story in its own right...
THE HUMAN BRAIN has several billion neurones all connected to each other and carrying nerve pulses to specific targets all over the body. A nerve impulse is an electrical activity that can be generated by the stimulation of a sensory receptor (taste, odour, hearing, sensation of pain, temperature, etc.) and sent to the brain for processing or, contrariwise, by the neurones to the organs.

At the cerebral level, the transmission of the nerve impulses from one neurone to another through the synapse is achieved by the release of neurotransmitters, such as acetylcholine, which can be captured by a receptor located on the next cell. The capture of a neurotransmitter then takes the form of a change in the conformation of the associated transmembrane ion channel which opens and closes, a bit like a switch, enabling the propagation of the nerve impulses.

How do the neurotransmitters activate the ion channels? What are the factors that favour or hinder their activation and the transmission of the nerve impulses? These questions are the focus of the research carried out by a team from the Macromolecules Structural Dynamic Unit (Unité de Dynamique Structurale des Macromolécules) of the Pasteur Institute, in collaboration with the team “Receptors and Ion Channels” of Pierre-Jean Corringer (Récepteurs et canaux ioniques) of the Pasteur Institute and researchers from the Institute of Physical-Chemical Biology (Institut deBiologie Physico-Chimique) at the CNRS.

“The feature of our laboratory is that it brings together experimental researchers and numerical simulation specialists”, Marc Delarue of the Pasteur Institute says. “Combining these two approaches has enabled us to both validate the experimental data and achieve a better understanding of it”, he added.

Based on the structures of the open ion channels identified using crystallography, the researchers were able to study two specific issues. Firstly, they were interested in the effects of certain substances such as anaesthetics and ethanol (found in alcoholic drinks and spirits) on the activation of the channel by the neurotransmitters: As these substances alter the emission of neurotransmitters and, in the long-term, the receptivity of the synapses, it is important to “identify how they work, notably how they attach to the receptors”, explained the researcher.

Secondly, they studied the mechanism for the passage of ions in the ion channel: “As these phenomena occur over a period of around a microsecond, we performed simulations that were as close as possible to that time scale. This enabled us to obtain results we could not have obtained before”, he explained enthusiastically. An ion channel is an extremely narrow and confined milieu, not a priori extremely favourable for the passage of hydrated ions: In facilitating this, the sides of the channel play a very active role in accompanying the ions all through their journey, right to the “exit”.

Thanks to these simulations “impossible to perform using just local resources”, the researchers were able to put together the first “realist film” of its genre. Following the work in 2012, these results were the subject, in February 2013, of an article published in the Journal of the European Molecular Biology Organization, the reference in the field of molecular biology (EMBO Journal).

Cross-section of an ion channel, lined with M2 helices (in grey). The extra-cellular part is at the top, the intra-cellular part at the bottom.

Selectivity of Ion Channels Involved in the Transmission of Nerve Impulses (CT7)
Principal Investigator: Marc DELARUE, Pasteur Institute
GENCI resource: Curie (CEA/TGCC)
JUST A MYRIAD of tiny bright spots as seen from Earth but a key role in terms of the Universe... The stars are of huge interest to astrophysicists because understanding how they are formed takes one back to the origins of the solar system and of its structuration, right up to the emergence of life on the Earth.

Stars are created by the accumulation of gas and dust in the form of clouds of molecules that condense and then collapse in on themselves under the action of gravitational forces. The gravitational collapse of these spheres of gas results in the birth of embryonic stars, protostars, surrounded on the outside by a belt of material known as the “accretion disk” and within which, in turn, aggregate celestial bodies. At the end of a period of “gestation” that can last for several million years, these protostars become stars, of varying sizes, around which planets circle: This is how a planetary system is born.

Whilst the general mechanism for the formation of stars seems well understood today, the processes at work are so numerous and so complex that they are not all fully understood by the astrophysicists. Thus, the magnetic field that stars often possess: Whilst we know how to measure it experimentally, we do not yet fully understand its exact role in their formation and those of the planets. It was the answer to this question that a team from CEA/Observatoire de Paris (Andréa Ciardi, Benoit Commerçon and Marc Joos) were looking for by studying, on one hand, the formation of massive stars, and, on the other, that of lower mass stars (like the Sun).

“The magnetic field is involved in the physical process of the star formation. Its action plays a role in controlling the speed of rotation of the gas by “braking” it, thereby facilitating the accretion between the various particles that make it up, and eventually, the creation of protostars”, as Patrick Hennebelle, astrophysicist at the CEA, explained. In the case of massive stars, the research team took an interest in the coupling between the radiation they emit and the magnetic field. It was a first: “Their interaction allows the increased focussing of the accretion and the formation of larger stars rather than a series of small ones”, he noted. In the case of the smallest stars, it was the conditions for the formation of the accretion disks that were analysed. “We carried out systematic studies on a large number of configurations (intensity of the magnetic field, angle of the magnetic field relative to the rotational axis of the star, turbulence, etc.) to explore the space of the parameters involved”, the astrophysicist explained.

“We were only able to achieve the degree of precision we were looking for thanks to the use of the national computing resources”, he added.

The work is continuing in 2013 using the Curie supercomputer with the aim of improving our understanding of how planetary systems evolve, obviously including our own.
Although it is nuclear fission that we currently use for our power stations, could nuclear fusion, more energy efficient but more difficult to control, be the energy source for tomorrow? The result of a huge international cooperation project, the International Thermonuclear Experimental Reactor (ITER), currently under construction in Cadarache, should help provide an answer. In the meantime, the scientists are getting ready for this huge experiment and improving their understanding of the physical phenomena involved. High performance computing is playing a key role in both aspects here.

“Our project is at the crossroads between theory, experiment and technology”, says Marina Becoulet, researcher at the CEA, in Cadarache. “ITER will have a radius of two meters, and we will be trying to looking at phenomena of a few millimeters. In addition, we will have to examine events lasting a millisecond in a period of several seconds, all involving a strongly non-linear physics: We need supercomputers for our simulations”.

Inside the fusion reactors, also known as ‘tokamaks’, the material is taken to a very hot state at which point the electrons become detached from the nucleus - referred to as plasma - and is confined by means of powerful magnetic fields. There are, within this plasma, magnetohydrodynamic phenomena with certain instabilities that, if not controlled, could seriously damage the reactors. In terms of ITER energy, they can melt tungsten in tens of discharges. The active control of these is therefore a matter of huge importance.

Using the Jade computer at the CINES, Marina Becoulet and her team have managed to simulate these nonlinear instabilities for realistic geometries such as those of ITER.

The project is part of a national and international collaboration between the CEA/IRFM, Inria, ITER Organisation, and JET (Union European), and based on the JOREK code.

Two methods for controlling the instabilities were identified. The first consists of injecting pellets into the plasma, with the aim of triggering weaker and thus less dangerous instabilities, and thus to extract the energy in small amounts. The other method involves varying the magnetic field by using coils with special properties that enable the suppression of these instabilities. In this latter case, the physics remains less well understood, thus explaining the level of commitment to developing both the theory and modelling in order to be able to produce predictions for the ITER.

The development of the JOREK code, as well as the power of the national computing resources, have made it possible to achieve unprecedented results. A basis on which the scientific community can advance its understanding of, and achieve optimised control over, fusion reactions.

Density (orange) and temperature (blue) at the edge of the plasma after injection of pellets at t=217

© CEA
Far from its apparent simplicity, light is an object with properties and behaviour that can be quite unexpected, most notably when it crosses solid material. This is especially true in the case of very high-power lasers, such as the Mégajoule laser (LMJ) of the CEA, near Bordeaux: An initial laser pulse is gradually amplified by optical systems, and it then has to pass through silica windows before reaching the centre of the installation’s experimental chamber. The propagation of the laser pulse in the silica generates significant damage, which we need to be able to fully understand.

This was the subject of the work of Luc Bergé, Director of Research at the CEA and Head of the Radiation-Materials Interaction Laboratory at the CEA (Laboratoire Interaction Rayonnement-Matière) and his team. When the laser pulse passes through a silica window it breaks down into small light filaments. This filamentation is a source of damage that is both optical (it destroys the homogeneity of the laser beam) and structural, because it generates a precursor plasma that will damage the material. “Controlling these phenomena is a critical stage for us to one day achieve fusion by inertial confinement”, Luc Bergé explained. “A tool was therefore needed that made it possible to model these and that is what we have done”.

This code, known as “SBS-3D”, makes it possible to simulate the propagation and the fragmentation of a laser pulse, both in time and in space, at scales that cover various orders of magnitude: A laser pulse lasting a few nanoseconds (several billionths of a second) generates by filamentation a singular amplification of the optical intensity as well as ionisation phenomena over much shorter times (several tenths of femtoseconds) and on very small spaces on all the materials. “This needed work using very large numerical tools consisting of several tens of billions of points, and therefore with a fairly long computing time”, the researcher said. In order to improve the quality of their results, the research team took on a new challenge in 2012: To adapt its code for graphic co-processors (GPU) which offer very large acceleration factors. Currently, the SBS-3D code is the first numerical tool in the world that can handle the various spatial and temporal scales, with “reasonable” computing times, of less than one week on 128 GPUs. “We have naturally made big improvements in terms of computing time, but also in terms of precision”, Luc Bergé pointed out. “With GPUs, the results of our simulations were obtained in four days, the same time as for a ‘conventional’ simulation with a resolution that is 16 times lower”, he added.

Their work on adapting the SBS-3D code for GPU technologies was recognised with the awarding of the second Bull-Fourier prize in 2012.

Nanosecond pulse simulations in 5 cm of silica. (a) The blue curves show the maximum intensity of the laser wave and the green curves that of the scattering under the Brillouin effect. The lighter colour curves indicate the limitations of the same computation performed on conventional processors. (b, c) Intensity profiles of (b) the laser pump wave and (c) the scattering wave simulated on GPUs during their propagation in the silica © CEA

Laser Filamentation Applied in the Production of Terahertz Sources and in Silica Glass Flux Resistance (CT10)
Principal Investigator: Luc BERGÉ, CEA - GENCI resources: Titane (CEA/CCRT) & Curie (TGCC)
**Materials**

**Tracking Defects**

All materials contain defects but these are generally in such small numbers that they do not radically alter their properties. In the case of nuclear power facilities or satellites in space, the natural or artificial radiation (radioactivity, cosmic radiation) to which they are subject can trigger defects that are more serious and with potentially catastrophic consequences. This means that it is therefore essential to have an accurate track of the creation as well as of the spread of any defects in the materials, in order to improve its resistance.

But what exactly is a defect? Under the effect of radiation, atoms move within the materials: They leave an empty space (a vacancy) or move into other atoms in so-called interstitial sites. In the case of semi-conductors, the problem is all the more critical as these materials are only imperfectly described by the Density Functional Theory (DFT), one of the most widely used methods today for calculating the structure of materials. Because, in properly identifying and monitoring defects triggered by radiation, we need to have an exact description of the material in question.

This is the challenge that was accepted by a team in the Physical Metallurgy Research Department (Service de Recherches en Métallurgie Physique) at the CEA (Nuclear Energy Division), whose work relates in particular to the analysis of the phenomena associated with the effects of radiation at the atom level: Applying another method, known as Random-Phase Approximation (RPA), to tracking defects in pure silicon. This was a scientific first because this method has been, up until now, mainly recognised for describing the dynamic of electronic systems: “Using this very well understood material, in 2012, we performed simulations on structures consisting of more than 200 atoms”, Fabien Bruneval, Project Manager, explained.

In 2011, this same CEA researcher had performed the same type of computing operation but on smaller structures, with just 64 atoms: the results of the series of simulations “were coherent and matched with the experimental data”, he pointed out.

These simulations, which had required “a great deal of computing time to achieve the necessary precision”, even made it possible to challenge an hypothesis stated by experimental researchers: “We showed that the diffusion of vacancies and interstitials has almost the same activation energy, whilst it had been thought that this was very different”, Fabien Bruneval pointed out.

These results were the subject of an article published in the Physical Review Letters, in June 2012, of a quality that was praised by the publisher. They represented a first step in “tackling more complex materials and of value in the energy field, such as silicon carbide”, the researcher added.

Another extension: The analysis of defects with an electronic charge (with more or with fewer electrons), which is a subject of considerable interest as some components, such as diodes, are produced by doping (selective addition of atoms) in semi-conductor materials.
THE GENERAL ATMOSPHERIC CIRCULATION MODELS used for weather forecasting or for climate studies all have the particularity of resolving synoptic scale “weather systems” (low-pressure or anticyclonic systems and frontal systems characterised by a spatial scale of around 1,000 kilometers and a timescale ranging between a few days and a week). These systems are spontaneously created by the instabilities in the circulation of air masses on a global scale, established by solar heating gradients that exist between the poles and the equator. They make a major contribution to the meridional movement of heat, humidity and the angular momentum.

The ocean also has “synoptic” systems dynamically comparable to those that exist in the atmosphere. These are eddies and “meso-scale” fronts characterised by a spatial scale of around 100 kilometres and a timescale of around a month. The largest part of the kinetic energy of the oceans (excluding the contribution of the tide) is contained in these scales. It was the space observation programme started in the 1990’s, namely the sea level altimeter observation programs (ERS1, Topex/Poseidon, etc.) that proved the omnipresence, in the world ocean, of these meso-scale structures. The central role in the dynamic equilibrium of the major current systems and the importance of their contribution to meridional movements of heat and properties as well as to the ocean biogeochemical cycles has, since then, been largely proven.

The explicit simulation of these structures in global oceanic circulation models has long represented a challenge in terms of the computing power needed. In effect, with characteristic scales 10 times finer than in the atmosphere, ocean models need, for an equivalent resolution of the dynamic, 100 times more grid points than for atmospheric models, which explains why the oceanic circulation models used so far for climate change studies have not yet explicitly resolved these scales.

“However, recent advances in the field of high performance computing and the availability to the scientific community of computers such as Jade at CINES, has enabled, by means of the refinement of the field, the development of very high resolution model configurations that explicitly resolve the meso-scale”, Bernard Bariier, Director of Research at the CNRS and researcher at the Glaciology and Environmental Geophysics Laboratory (Laboratoire de Glaciologie et Géophysique de l’Environnement, LGGE) in Grenoble, explained.

This exceptional degree of accuracy enabled the researchers to advance their in-depth understanding of the ocean, in particular of the Atlantic Meridional Overturning Circulation (AMOC) which plays a key role in

Snapshot (5 day average, centred on 01 December 1992) of the surface current speed module (at a depth of 3 meters, units = cm/s) produced by a DRAKKAR simulation using the ORCA12 model. The maximum speeds exceed 1 m/s. The sea ice cover is shown in white. The drag and the meanders of the major oceanic currents as well as the tropical wave and the multitude of oceanic eddies in all the regions of the ocean can only be seen with the very high resolution made possible using the resources of GENCI.
the climate changes that have occurred in the past 20,000 years.

This large scale oceanic circulation, which can be “ON” during interglacial periods and currently, or “OFF” during the glacial periods, influences the climate because it contributes, with the atmosphere, to carrying the heat received at the equator towards the poles. The transition from one state to the other is extremely non-linear, thus explaining the sudden changes that occur in the AMOC status.

“Until now, future climate simulations all predicted a slowing in the AMOC but without any sudden change in state. Now, thanks to the performance of realistic oceanic simulations with greater spatial resolution, we have shown that a sudden change in the AMOC is possible under current climatic conditions”, Julie Deshayes, researcher at the Ocean Physics Laboratory (Laboratoire de Physique des Océans, CNRS), noted. “These were ground-breaking simulations and the joint performance of four long simulations (two on GENCI resources, one in Germany and one in Great Britain) made it possible to check that this result is robust despite the intrinsic uncertainties of the simulations, in terms of atmospheric conditions or certain ocean model parameters, for example”, she confirmed.

These results, which have been submitted for publication in the Geophysical Review Letters, one of the leading scientific publications in the climatology field, also highlight the need to increase the resolution of oceanic models in order to better reproduce the impact of meso-scale processes on the circulation and the average characteristics of the water mass, and thus reduce the gap with observations, but also for a better integration of the effects produced by strongly non-linear processes. “In the context of the stability of the AMOC”, Julie Deshayes said, “there are processes associated with salt exchanges between the South Atlantic and the Indian Ocean, which require high spatial resolution in order for us to correctly reproduce these”.

These simulations were performed as part of the DRAKKAR project with the ORCA12 configuration. “This is a new global configuration of the ocean/sea-ice circulation model, NEMO, with a horizontal resolution of 1/12°. It uses a computing grid with a step that varies from 9 kilometres at the equator to less than 3 kilometres across the Antarctic continent; which represents, with 46 vertical levels, just over 0.6×10^9 computing points. Following the scalability analysis, a computing subject-field analysis using 3,000 processors enabled the performance of an 85 year simulation in two months of time, using GENCI resources”, Bernard Barnier described.

But the search for high resolutions does not just meet the needs of researchers; it is also driven by the need, for operational oceanography, to deliver real-time analyses and predictions of the state of the ocean. ORCA12 is used by the Mercator Ocean operational oceanography centre for its real-time forecasts.

DRAKKAR Project (CT1)
Principal Investigator: Bernard BARNIER, CNRS
GENCI Resources: Ada (CNRS/IDRIS) & Jade (CINES)
Oceans play a fundamental role in the thermal equilibrium of the Earth and their interaction with the atmosphere is the key to the evolution of the climatic system. This system can be compared with a huge heater, regulated by the exchanges between the atmospheric (the winds) and oceanic circulations (the currents). Improving our understanding of the ocean is thus essential in establishing reliable predictions of medium and long-term climate change. This does, however, presume that we have as precise a model of the ocean as possible.

A model of the ocean is a representation, in the form of equations, of all the physical and biogeochemical processes that take place within it and the interfaces with other terrestrial components (atmosphere, continents, etc.).

That was the challenge for the work on data assimilation undertaken by Didier Auroux and his team at the University of Nice Sophia Antipolis (UNS). Applied to the NEMO modelling platform (Nucleus for European Modelling of the Ocean) which calculates the state and the evolution of the ocean for both seasonal and climatic forecasting, this approach involved the coupling of the results of the simulation and the data from satellite (pressure and surface temperature) and in-situ observations (temperature and salinity profiles) to determine the “right trajectory” for the model, i.e. to adjust it as accurately as possible in order to get a realistic prediction of how the oceans will change, in this instance the North Atlantic.

“For this work, we used a specific algorithm, BFN (Back and Forth Nudging), which was developed in our laboratory in collaboration with Jacques Blum and compared with other methods by Giovanni Ruggiero”, Didier Auroux explained. This algorithm makes it possible to resolve equations in the model in the time intervals where satellite data is available, by performing back and forth nudging on these periods to achieve a gradual convergence, by means of using a “feedback term”, between the model solution and the data.

“These are fairly large scale problems”, the researcher told us. “We have a million variables to take into account, a number of physical variables (such as pressure, temperature, salinity, etc.) but dispersed through a space (for instance, different ocean depth levels) represented by a grid with several thousand points. This means we need a huge amount of computing power and this can only be supplied by national resources. We used the Vargas computer at IDRIS to perform our computing”.

The results? “There were very good”, Didier Auroux enthused. “With our algorithm, much simpler to use than the others, we achieved a better estimation of the ocean than those managed so far because it was more consistent with the observations”. Offering some comfort for climate specialists in their search for reality...
Analysis of the dispersal of bubbles in the flow of a fluid contained between two rotating cylinders. On the left, we can see the structure of the flow in correlation, right, with the position of the bubbles.

**Principal Investigator:** Dominique LEGENDRE - Institut de Mécanique des Fluides de Toulouse (IMFT)

**GENCI Resource:** Jade (CINES)

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Simulation of a supersonic hydrogen flame. ONERA/LAERTE Experiment

**Principal Investigator:** Ivan FEDIOUN - Institut de Combustion Aérothermique Réactivité et Environnement (ICARE), Orléans

**GENCI Resource:** Vargas (CNRS/IDRIS)

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Visualisation of water saturation in an underground reservoir

**Principal Investigator:** Benoit NOETINGER, IFPEN

**GENCI Resource:** Curie (TGCC)
**Simulation of a 7 mm layer of oil subject to vibrations at 10 Hz**

**Principal Investigator:** Damir JURIC, Laboratoire d’Informatique pour la Mécanique et les Sciences (LIMSI) UPMC/Paris Sud.

**GENCI Resource:** Babel (CNRS/IDRIS)

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**Formation of a magnetised wind on the surface of an accretion disk**

The colours represent the density of the gas and the tubes represent the lines of the magnetic field

**Principal Investigator:** Geoffroy LESUR, Institut de Planétologie et d’Astrophysique de Grenoble

**GENCI Resource:** Vargas (CNRS/IDRIS)

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**Simulations of the evolution of a spiral galaxy similar to the Milky Way, including dark matter and the baryons, and computing the formation of stars, the metallicity and the feedback**

**Principal Investigators:** Françoise COMBES & Paola DI MATTEO, Observatoire de Paris

**GENCI Resource:** Curie (TGCC)
Formation of clusters on a random fractal near the critical point of the ferromagnetic transition

**Principal Investigator:** Pascal MONCEAU, Laboratoire Matière et Systèmes Complexes (CNRS)

**GENCI Resources:** Vargas (CNRS/IDRIS) & Jade (CINES)

Non linear fast MHD plasma relaxations modeling in existing tokamaks and ITER

**Principal Investigator:** Marina BECOULET (CEA)

**GENCI Resource:** Jade (CINES)

S2D simulation (using the CALDER particle code) of the interaction between an ultra-intense laser pulse (intensity of 1020 W/cm²) and partially extended aluminium target (as a result of an initial lower intensity laser pulse). The colour chart measures the local density of the kinetic energy of electrons with an energy greater than 100 keV (in units of 511 x 1021 keV/cm³).

**Principal Investigator:** Laurent GREMILLET, CEA/DAM Ile-de-France

**GENCI Resource:** Jade (CINES)
Numerical modelling of the magnetic environment of the Sun using data for three components of the magnetic field in the solar photosphere, measured by the Heliosismic and Magnetic Imager at the Solar Dynamics Observatory and the MESHMHD code

**Principal Investigator:** Tahar AMARI, Centre de physique théorique (École Polytechnique)

**GENCI Resource:** Vargas (CNRS/IDRIS)

Fullerenes in lipidic membranes

**Principal Investigator:** Luca MONTICELLI, Dynamique des Structures et Interactions des Macromolécules Biologiques (Inserm)

**GENCI resource:** Jade (CINES)
High resolution simulation of nonlinear dispersive partial differential equations

Principal Investigator: Christian KLEIN, Université de Bourgogne
GENCI Resources: Vargas (CNRS/IDRIS) & Jade (CINES)

Non vanishing transverse dispersion in 3D heterogeneous porous media

Principal Investigator: Anthony BEAUDOIN, Université de Poitiers
GENCI Resources: Vargas (CNRS/IDRIS) & Jade (CINES)

Special thanks to:

Carlo ADAMO (Chimie Paris-Tech), Jean-Michel ALIMI (CNRS), Didier AUROUX (Université de Nice Sophia Antipolis), Édouard AUDIT (CEA), Marc BAADEN (CNRS), Éric BARAT (CEA), Bernard BARNIER (CNRS), Marina BECOULET (CEA), Luc BERGÉ (CEA), Jacques BLUM (Université de Nice Sophia Antipolis), Frédéric BOUSSER (Université de Corte), Fabien BRUNEVAL (CEA), Francis DAUMAS (CINES), Marc DELARUE (Institut Pasteur), Julie DESHAYES (CNRS), Jean-Baptiste FILIPPI (Université de Corte), Denis GIROU (CNRS/IDRIS), Patrick HENNEBELLE (CEA), Sylvie JACQUEMOT (École Polytechnique), Catherine LE LOUARN (GENCI), Marie-Bernadette LEPETIT (CNRS), Patrick MASCART (Observatoire Midi-Pyrénées), Thierry MASSARD (CEA), Christine MÉNACHÉ (CEA), Thierry MONTAGU (CEA), Olivier PIRONNEAU (UPMC), Alain PASTUREL (CNRS), Stéphane REQUENA (GENCI), Giovanni RUGGIERO (Université de Nice Sophia Antipolis), Yves-Henri SANEJOUAND (Université de Nantes), Marc THIRIET (Inria), Luc VERVISCH (CORIA).