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SIMULATION BIG DATA HPC IA

Report Plenary Session





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Forum Teratec 2020 : **HPC, AI and Quantum** computing remain as central matters for industrialists and Europe

The Forum Teratec being organized remotely this year using video conferencing was a real opportunity for speakers to show how HPC and digital simulation often coupled with Artificial Intelligence applications can be used to fight the pandemic, by anticipating its progression and accelerating the development of new drugs. Many other examples were equally presented from the Defense or Energy sectors. Finally, this year's event was also an opportunity for European Commissioner Thierry Breton to reassert Europe's determination to come back as a world leader in HPC equipped with some of the most powerful supercomputers in the world and able to develop in Europe all technologies required, whether in terms of processors, software, exascale architectures or quantum machines.

Due to the **Covid-19 epidemic**, the **Forum Teratec 2020** annually planned in June was postponed to October 13 and 14 then, unfortunately it had to be held remote due to health restrictions.



Panel of Speakers for Plenary session were comprised of:

Daniel Verwaerde President and co-founder of **Teratec**

Thierry Breton European Commissionner

Florence Parly Minister of French Armed Forces

Alain Rousset President of Regional Council - Nouvelle-Aquitaine

Xavier Ursat Executive Director Groupe EDF

Marie-Noëlle Semeria Director of Research and Development Groupe Total

Éric Genevois-Marlin global Head of R&D Digital and Data Sciences de <mark>Sanof</mark>i

Trish Damkroger Vice President Intel Data Center Group

Kevin D. Kissell CTO Google





Thus, in a video recorded message of about ten minutes, each of the speakers addressed main topics which are outlined below.



Daniel Verwaerde, president and co-founder of **Teratec**, opened the **Forum Teratec 2020** recalling that the Covid-19 epidemic initially led to shift the event from June to October, eventually to be converted into one *digital event*.

« Its quality will have been met as well since its program has been entirely maintained, bringing together industrial users (**EDF, Total**, **Sanofi**) to express their vision of HPC development in their sectors, but also some of the most advanced technology providers (**Intel**,

Google) unveiling their roadmap both in the field of components and future uses, alike major policy makers (**Thierry Breton**, for the European Commission; **Florence Parly**, Minister of the Armed Forces; **Alain Rousset**, President of the Nouvelle Aquitaine Region) ready to share their vision of digital technology intended to be implemented. So I encourage you to watch their videos.»

Three major prospects

Then, he reminded about this epidemic having increased the fundamental importance of digital technology, and especially **HPC** [*High Performance Computing*] and **HPDA** (*High Performance Data Analysis*) in our lives and our economy, particularly in healthcare. According to him, the future of these technologies will be shaped by three major prospects: the recovery intended by most States thus placing the emphasis on digital; the rise of Europe in the field of digital technologies; and rapid progression of future technologies, particularly quantum computing which may well be one of the major technological breakthroughs of the coming decade.

Teratec's action

He also highlighted Teratec's role in this changing world: «Over the past year, our actions have been aimed at establishing France within the European HPC and HPDA community. We have pursued three lines of work: actively participate in the governance of **EuroHPC** in order to represent French interests; spearhead the creation of the French Competence Centre alongside **GENCI** and **CERFACS** to provide broad support to companies, so that they can fully benefit from resources made available by the European Union; involve European manufacturers in this major EuroHPC project by creating a federation of companies to formally represent them."

Quantum computing will put European HPC back on track

Daniel Verwaerde concluded with describing his vision of quantum computing: "The coming decade will see a technological breakthrough thanks to quantum which will revolutionize the way to compute. Progress made over the last few years will make it possible for first computers and accelerators to be operational by 2025/2030. This is a real opportunity because France is leading the race, and since any technological revolution is about to reconfigure the world stage, this will enable Europe to come back in a leading role after a period of almost 70 years with a follower rank in HPC."







Second much-awaited intervention was that of **Thierry Breton**, **European Commissioner** for the Internal Market. He also reminded that the Covid-19 pandemic demonstrated the fundamental importance of digital technologies in our lives, before insisting on Europe's involvement in HPC and in other related technologies.

« I see the coming decade as the digital decade in which Europe can become a leader on the global technology scene. There are several reasons for this. First, all economic sectors and human activities depend on digital technology today. To analyze all this data, to make it useful to

our business, we need to strengthen our capabilities in High-Performance Computing, but also in Artificial Intelligence, Big Data, Cloud, Edge computing...»

HPC as one of the key pillars of Europe's digital autonomy

He went on to emphasize Europe's commitment to HPC: « *High-Performance Computing is now making it possible to solve very complex problems in a number of essential application areas for Europe today (personalized medicine, energy, engineering, chemistry, exploration for oil and gas, cosmetics, materials, climatology, cyber-security, defense...).* This is a major strategic challenge for Europe, as much industrial, technological as scientific. It is one of the pillars of our digital autonomy. This is why the European Commission has proposed to Member States to include HPC *in their massive investment plans part of* **Next Generation EU** - the European Union's package of economic recovery measures. All Member States will devote a minimum of 20% of their national investment plans to digital. This will represent more than 130 billion euros over the next 2 to 4 years. This is a major boost for Europe's digital decade. And on September 18, the European Commission also proposed to invest, *together with Member States and industry, more than 8 billion euros in exaflopical supercomputers within EuroHPC Joint Undertaking.*»

EuroHPC, 8 billion Euros for HPC

These investments will serve many purposes. « These plans are in line with the Union's strategy. Launched in 2018, EuroHPC is in the process of acquiring eight world-class supercomputers, 3 of which should be in the Top5. These machines will multiply the computing power available in Europe by a factor scale of 8. They will be available to all users, including universities, the public sector, industry and especially SMEs, wherever they are in Europe. »

« The investment plan announced on September 18 will be used to acquire and deploy new-generation supercomputers with exaflopic capacity, and to invest in partnership with manufacturers to acquire machines adapted to their needs and quality of service; to interconnect all these machines via Terabytes networks; develop and master the underlying technologies of supercomputers, in particular by investing in low-power



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>>> consumption processors, a key technology for exaflopic machines, but also for autonomous cars, smart phones, Edge Computing or Cloud servers, etc. So it is a matter of Europe's digital sovereignty. »

Meeting the challenge of quantum computing and processors

He then addressed major challenges facing Europe, namely quantum computing and processors. « Finally, we need to move beyond HPC and in particular towards quantum computing, as next technological challenge of this century. Quantum computers will be able to process huge datasets to solve problems that were previously inaccessible to today's best performing machines. Even before the arrival of supercomputers, this quantum revolution will begin with the introduction of accelerators dedicated to specific algorithms by adding cards to traditional supercomputers.»

« Beyond supercomputers, European sovereignty will also be conditioned by Europe's ability to produce the world's most powerful processors, in order to reduce our dependence on such strategic technologies. We have technological and industrial capacity to do this, as well as one common political will. We are therefore preparing to launch one European industrial alliance for microprocessors around the **Ecsel j**oint venture with very substantial funding.»

Learning to collaborate

« My final message will be a call on European cooperation to make our vision of the digital decade a reality and to guarantee Europe's digital autonomy. We need to build European technological ecosystems bringing together all stakeholders, research organizations, small and large companies, and of course public authorities. We need to learn from each other, identifying our weaknesses and strengths on which to build it all, and this Forum Teratec is obviously one excellent opportunity to take this collaboration forward. »









Another key intervention was made by **Florence Parly**, **French Minister of the Armed Forces**. She recalled the interest of digital technologies and the enabled disruptive innovations benefiting to her ministry.

« I wanted to speak in today because Artificial Intelligence, High-Performance Computing, Quantum computing and, more generally, disruptive innovations linked to digital technology and data, are subjects of utmost importance for the French Ministry of the Armed Forces. The Ministry of the Armed Forces has always established itself as one key player in these cuttingedge technologies which remain central facing the challenges

of technological and industrial sovereignty, whether at national or European level. Therefore, these are also at the heart of our innovation strategy and our investments, with the aim of devoting 1 billion euros a year as of 2022.»

Playing synergy between civil and military sectors

A race for innovation is on today driven by the civilian world, on which the defense industry must rely. « One of the areas with a lot to gain from exchanges with the civilian world is obviously AI, one key technology for us. Today we are facing genuine digitization of the battlefield and the emergence of connected and combined combat. Our weapons and equipment have evolved a lot with on-board sensors, and today they generate massive use of data. This is why we have developed a roadmap for defence AI in 2019. During the 2019-2025 military programming law, 100 million euros will be invested each year on average and nearly 200 data scientists and other experts in this field will be recruited by 2023. »

Relying on industry and research

« One of the flagship projects of this roadmap, called **Artemis**, aims to provide the Ministry of the Armed Forces with a secure and sovereign info-structure for massive data processing. This project will help pool the mass of data produced within the Ministry, and facilitate its management, administration and use. The developments made for this tool will, I hope, serve as building blocks for applications beyond the defence sector. This is why I wanted our strategies in terms of AI and quantum technologies to rely on a variety of partnerships with industry, SMEs and start-ups, but also with the entire research ecosystem, including **INRIA**, **CEA**, **CNRS** and **ANR**. A call for projects has also been launched with the ANR on quantum technologies, with the aim in particular of ensuring the integration of quantum accelerators in computing centers. »

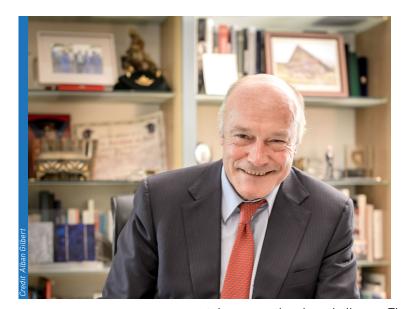
Bringing European complementarity into play

In conclusion, she insisted on the fact that we have research laboratories, technology suppliers and manufacturers in France and Europe capable of developing new applications and European projects in this area, such as **EuroHPC**. « It is the emergence of this European approach in key technologies, driven by **Teratec** that we will need to collectively support both for government and industry. Let me assure you that the French Ministry of the Armed Forces, through its industrial and innovation policy, is scrupulously watching over this relying on your know-how. »

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For the last speech among invited political decision-makers, **Alain Rousset**, **President of the Regional Council of New Aquitaine**, stressed the complementary nature of actions to be carried out at European, national and regional levels.

« France is well placed in the fields of High-Performance Computing, Big Data and Artificial Intelligence. However the challenge of acceleration of technologies is leading us to

take up another key challenge. This means we need to think on a European scale. Nonetheless, we are also investing at regional level in multiple research structures and in very high-speed networks.»

And such Research covers many sectors, while giving some examples. « In our region, we have platforms dedicated to health with oncology, materials chemistry, even on animal health currently making extremely strong contributions. We are also working on the agro-ecological transition, where we are carrying out a project called **VitiREV** with many operators, helping to remove pesticides and glyphosate from the vineyards. The use of AI and HPC allows us to quickly assess the impasses that farmers and winegrowers are encountering, in order to accelerate this transition.»

« We have similar AI devices in the field of cancer treatment allowing us to compare the DNA of individuals with great efficiency in many hospitals around the world, in order to better manage medical responses to specific types of cancer. The same is done in cardiology as it is in neurology. »

To meet these challenges, the Region of New Aquitaine is going to install one Big Data secured platform to facilitate exchanges in terms of biosecurity or cybercrime. « We are counting on your work to enlighten public authorities and businesses in these areas, as much essential, critical as sovereign.» he concluded.







As the first industrialist to speak, **Xavier Ursat**, Executive Director of the **EDF Group**, explained how HPC and digital simulation contributed to improving the safety of the group's industrial facilities.

« High-Performance Computing and Artificial Intelligence are widely used in our industry, and we are investing heavily in them. We are almost doubling our computing power every two years to reach 7 PFlops today, making us one of the five largest supercomputing operators in France. We also have a quantum computer from Atos with 120,000 processors that bring even more computing capacities."

These high-performance computing capabilities are vital for us, because we must always increase the safety of our nuclear reactors and provide ever greater precision in the studies required of us by the Nuclear Safety Authority. This requires a lot of simulations and therefore a lot of computing power. »

HPC increases the security of our installations

Such computing power also makes it possible to use the billions of data recorded over decades in nuclear reactors and hydroelectric facilities to serve simulations based on this feedback.

"We have also been able to strengthen our fuel assemblies based on Machine Learning algorithms, which enabled us to optimize all the parameters to guarantee both better performance and greater safety."

Finally, computing capacity is used to simulate the behavior of equipment under extreme conditions, which improves operator responsiveness and increases the safety of installations.

2000 HPC users

Today HPC and AI allow EDF to make new qualitative leaps. For example, it uses complete digital twins of its nuclear production fleet, to train power plant operators in such conditions very close to the reality of operation, and simulate the evolution of the various components over time in order to optimize their maintenance. These technologies utilizing Machine Learning software are also used to simulate the balance of production facing the evolutions in electricity demand scenarios. He also confirmed that EDF is already working on adapting its models to future quantum machines. Nowadays, more than 2,000 engineers within EDF use these HPC resources, including around 800 staff working in R&D.

Preparing the electrical system of the future

And to conclude about the challenges of the electrical system of the future that HPC should help to meet: « More than ever before, the challenges of the electrical system of the future will require these resources in HPC. New decentralized and centralized means of production, new forms of consumption, as the challenges of constantly adapting to climate change, make these tools essential. We are working hard on this, and that is why the EDF Group will be present and will be able to meet the challenge of computing power."»







Second presentation made by an industrialist with **Marie-Noëlle Semeria**, Research and Development Director of the **Total Group**, who explained how digital technologies could help the oil group to ensure its transformation into a multi-energy company.

« Our objective is to increase the share of electricity from 5% today to 15% in 2030, while fully integrating climate issues and aiming for carbon-neutral production in Europe by 2050. We can do this by working on tools, software, and solutions brought to the global system, either to diversify the contribution by using green energy, or by recovering and storing CO². These challenges lying ahead require highly significant computing capabilities along with all HPC expertise.»

HPC accelerates our mutation

She then gave some examples of how these technologies are being used in the group: CO² capture with the challenges of molecular modeling to find the most efficient material; geological storage of CO² with the challenges of simulation on fluidic and mechanical aspects; optimization of giga-farms, either offshore wind turbines or solar installations, hybridization of networks; optimization of electric vehicle fleets, etc.

« In all these areas we generate large amounts of data, and thanks to simulation coupled with AI we can now increase our learning speed tenfold by developing predictive models and being able to model complex systems that are not observable. We keep following the scientific approach described by Descartes, but with a formidable acceleration enabled by all the capabilities of high-performance computing, data science and, more generally those of digital technologies.»

Al is a real "Game Changer"

« In the field of AI, we have to develop increasingly complex algorithms that require more and more computing capacity, and that's where HPC comes in to give us this capacity, to generate predictive models more quickly and support learning over time, to maintain their reliability. Distributed intelligence models are a real 'game changer' because they enable us to address three challenges: performance, with design of the computing architecture to optimize what is being done as close as possible to the field and only trace what is necessary, energy efficiency since we are limiting our carbon footprint, and third, the issue of sovereignty by keeping the data as close as possible to the sites. The value of industrial data starts already in the way it is processed, as close as possible to measurement, hence the challenge of Edge Computing and 5G technologies which are fully part of the HPC roadmap. »

Assessing the interest of quantum

But the Total Group goes a step further: "Beyond classical methods, new fields such as quantum are opening up. We want to be present and active in these fields, to be able to formalize our specific issues in the right quantum language. This technology has tremendous potential because it allows us to accelerate everything that is parallel by investing on the superposition and entanglement of quantum states. We are already using a quantum computing emulator from Atos to learn from it."

She concluded: « Digital technologies are an asset for Total, an accelerator of transformation, a catalyst in relation to 5G technologies, Edge Computing, and a formidable generator for innovation, because the most exciting is what these technologies will enable us to discover in multiple areas (materials, systems, processes ...).»

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Last industrialist speaking was, **Eric Genevois-Marlin**, Global Head of R&D Digital and Data Sciences at **Sanofi**, who explained how digital technologies are fundamentally transforming the process of creating new drugs.

« Bringing a new drug to market today requires 8 to 10 years of R&D, hundreds of employees and a budget ranging from 1 to 2 billion euros. We want to improve that. We are focusing our R&D efforts on several

specific therapeutic areas: cancer; immuno-inflammatory diseases; hemophilia; rare diseases; viruses, including Covid-19. Therefore, we need to study these pathologies, their complicated biology with multiple variants, the many patient populations and different phenotypes, in an extremely precise manner. »

And to explain that R&D in this field calls upon many sciences (biology, chemistry, physics, chromatography, medicine, engineering...) but also lots of mathematics (probability, statistics...) and now Artificial Intelligence.

Deep Learning selects molecules faster

« Today we are assessing the use of Deep Learning coupled with HPC in research, to find in the space of chemical molecules (with size order of 1060 to 1080) a subset of molecules that would have the desired chemical properties, as well as the capacities in terms of activity and tolerance in order to meet the expected therapeutic needs. We are also working on the application of this type of method on biological molecules from cell culture, in order to produce an antibody that will be able to attack an antigen known to be responsible for a given pathology. This is a considerable area of innovation that has opened up, for which we hope to record interesting results in the near future.»

AI to better target clinical trials

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Al is also widely used in the human testing phase. « We are testing a Deep Learning algorithm to study cell images from patients to accurately identify and measure their exposure to a particular antigen. We will target this antigen with an antibody based on one of our molecules. This exercise will allow us to predict the activity of our product. To do this, we will simulate clinical trials using traditional methods (randomized trials) with typical analytical methods (Cox regression model). We will deduce the degree of probability that a clinical trial conducted for these patients will be conclusive. This has not been done yet, but this approach would make it possible to target with great precision the patient population we wish to treat, being almost certain of the effectiveness of the treatment.»

Numerical technologies have also been widely used at Sanofi to build predictive models by processing data collected in real time via sensors. They are used to evaluate and optimize manufacturing processes to facilitate more accurate decision-making. Finally, these technologies are also used to manage the considerable volume of knowledge accumulated by Sanofi over decades.





>>> An industry undergoing profound change

Using digital technologies implies a profound change in the pharmaceutical industry. « Over the last 5 years we have seen registration authorities in major regions of the world (Europe, USA, China, Japan) starting to adopt these new techniques to evaluate new molecules discovered on the basis of AI algorithms. In the coming years, this will induce a profound change in the pharmaceutical industry and its R&D because data, technique, methods of analysis and computing capacity will have fundamentally transformed the intellectual process leading to the creation of a new drug.»









The plenary session concluded with the presentations from two leading technology providers. **Trish Damkroger**, Vice President of **Intel Data Center Group**, explained how the processor manufacturer is adapting its products to be at the heart of HPC/IA convergence.

« The role of digital technologies has never been more apparent than during this pandemic, both trying to find cures but also keeping schools and businesses running, with distance working on a scale previously unimagined. Thanks to the rise in cases of using AI, many teams are entering a new era of computing and modeling. The convergence of HPC and AI is accelerating many simulations, and models created by AI are replacing traditional models. »

An architecture fitting IA / HPC convergence

« To support this convergence, we developed the **Intel XPU Strategy.** It mixes CPU, GPU, FPGA and specific accelerators, with Deep Learning at Data Center and Edge Computing levels, all around one unified standard programming open model. The objective is to simplify application development and their portability. »

« Convergence between HPC and AI is the critical inflection point for the HPC industry and Intel is one of the key partners to achieve this. Our **Xeon** processor is optimized for this with **Advanced Vector Extensions 512** which accelerates HPC applications, DL Boost accelerating AI applications, and **Optane** persistent memory accelerates Data Analytic and AI applications. While the 2019 **Cascade Lake** version of our Xeon processor in 2019 used 14nm engraving technology, this year's **Ice Lake** version uses 10nm technology and the 2021 **Sapphire Rapids** version will see a new generation of DL Boost with Advanced Metrix Extention (**AMX**). On the GPU side, the **Xe** architecture is very versatile, adapting from conventional machines to supercomputers, from TFlops to exascale. The new **PonteVecchio** processor using 10nm technology will be dedicated to HPC machines. »

« We have also worked across the ecosystem to develop **oneAPI** to facilitate programming across multiple types of processors, accelerators and CPUs, GPUs or FPGAs, whether processing scalar, vector, matrix or spatial data.»

« So we are ready to help you build a future made convergent, whether be processors, architecture, memory, interconnection, security or software. »







Last speaker invited, **Kevin D. Kissell**, CTO of **Google**, who described how hybrid solutions are the most effective way to adapt to the complexity of a changing world.

« The deployment of hybrid HPC/Cloud solutions, combining local HPC infrastructures with resources in the Cloud, is already working, for example in the field of high-energy physics. As early as 2016, we helped **FermiLab** double the number of processor cores accessible via the **HEPCloud**, the Cloud of the particle physics community, by connecting it to our Cloud via **HTCondor**. In 2019, we helped **CERN** replicate the Higgs boson discovery using Kubernetes technology.

This Open Source system provides a platform to automate the deployment, scalability and implementation of application containers on server clusters. It was used here with our Google Container Engine (**GKE**) to process 70 TB of data using 20,000 virtual processor cores.»

Blending Machine Learning and HPC

He also gave another example of hybridization in the field of weather prediction where the **Google Brain Research Team** worked for the **NOAA** (National Oceanic and Atmospheric Administration). They replaced the traditional physical simulation with optical analysis of satellite images to produce precipitation forecasts. Operating on a neural network of more than 256 Google TPU, this model called **MetNet** proved to be much more accurate and much faster than traditional simulation.

Quantum goes with hybridization

He explained that in the field of quantum computing, there are also hybrid applications mixing variational and classical methods. Thus a parametric quantum model of a system can be optimized iteratively using classical algorithms. « *This year, this allowed us to model the diazene H2N2 molecule with sufficient precision to simulate the formation of the two isomers in Cis and Trans, on one of our* **Sycamore** *processors. This is an important advance that shows the interest of quantum computing in the field of science.*»

Kevin Kissell also presented other hybrid applications in the management of major climatic disasters to anticipate and organize preventive evacuations of affected areas, or the calibration of neutrino detectors in physics.

« Hybrid solutions combining numerical simulation, AI, HPC, quantum, Cloud, etc., are of clear interest in many fields. They offer more processing possibilities, more power to deal with increasingly complex problems more quickly. This will be the solution to meet the challenges of the future in the fields of health with pandemics or climate change.» he concluded.

Jean-François Prevéraud