HEADLINES:

Numerical simulations in materials science

Cancer research
Attracting young talented students to science

Like most scientific universities in developed countries, we are witnessing a growing trend among talented students to pursue studies in areas other than basic science.

Two reasons may be invoked to explain such a lack of interest. Firstly, educational scientific programs in secondary schools may need to be updated and reconsidered with a new pedagogical approach. Secondly, the period of time required to access a job in science may appear as excessively long. In France, for example, eight years are needed after the baccalaureate to obtain a PhD degree. To this, one must often add two additional years of post-doctoral studies abroad, before becoming potentially eligible for a stable academic research position.

Our University is currently endeavouring to change such a situation. Priority actions directed toward young students are being engaged to stimulate their interest. These include both specific informative meetings, organized in secondary schools and during open days at the University, to explain the reality and benefits of scientific studies. In addition, a growing number of new diplomas with specific professional orientation are currently being created at the intermediate levels of License (degree) or Masters degrees, thus offering new opportunities for students to enter a professional career earlier, notably, between just three and five years after their baccalaureate.

The first headline of the present issue of our magazine deals with the utilization of numerical simulations as a reliable complementary tool for exploring the properties of matter. This is a field undergoing intense development, particularly with the advent of nanosciences. It is also a multidisciplinary research domain in which several laboratories in Toulouse are involved.

The second headline deals with oncology. Cancer research is indeed a very important part of medical research. We present a new organization known as the "Toulouse Oncopole", in which outstanding fundamental research in cancer is directly in line with transfer of knowledge and clinical treatment, in collaboration with industry.

Let me wish you pleasant time with our scientific magazine.

Gilles FOURTANIER
President of Paul Sabatier University
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http://www.ups-tlse.fr/27503789/1/fiche__pagelibre/&RH=rubrech03
Exciting new materials can now be grown or synthesized with very good atomic and chemical structures. Some of these materials do not even exist naturally and can only be obtained in research laboratories, by clever manipulation of matter at the nanometre scale. These materials possess unexpected physical properties. They are currently the object of fundamental investigations with the aim of understanding the origin of their interesting behaviour. These materials can be used for technological applications in various fields like bio-nanotechnologies, microelectronics, magnetic memories and structural materials.

Supercomputer
Numerical simulations must be used to understand the microscopic origin of the physical properties of these materials and to interpret results of experimental studies on these systems. These simulations are complicated because we usually need to describe the behaviour of a huge number of electrons and nuclei interacting together. The mathematical equations describing the physical properties of these materials can only be solved with a supercomputer like the one provided by CALMIP (Calculations in Midi-Pyrénées). The researchers of the main laboratories in Toulouse studying the physical properties of materials (at CEMES¹, CIRIMAT², LAAS³, and laboratories belonging to the IRSAMC⁴ institute) routinely use this kind of computer.

Each year, these laboratories apply for calculating time on the CALMIP computer and about 30 research project proposals are submitted each year. In 2011, CALMIP allocated 5 000 000 hours to these labs for calculating the physical properties of materials. This represents 22% of the total available calculation time. The codes that calculate the physical properties of materials are well suited to massively parallel architectures and run on Hyperion, the most recent supercomputer at CALMIP.

We can also mention the case of calculations to study an Fe nanocube: the use of 256 processors means that one calculation loop can be performed in just 30 seconds (this is important since convergence requires thousands of loops). The active collaboration between CALMIP technical staff and new users with little experience in numerical calculations and computing allows to parallelize the codes that they have developed. This has been the case for a code written for studying the electromagnetic properties of nano-objects using more than 200 Go of shared memory. To carry on meeting such needs and further increasing computer capability, CALMIP will acquire several hundreds of processors and several TeraOctets of shared memory in 2012, in the framework of the EQUIP@MESO (EQUIPEX) project.

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CALMIP and the Hyperion supercomputer:
Thanks to the active support of UPS, and in collaboration with the PRES University of Toulouse, CALMIP is able to provide a high-performance calculation platform to the local scientific community. Hyperion (2912 cores, 33 Teraflops) was acquired in 2009 thanks to CPER funding. This computer is hosted and managed by the DTSI staff (head office for information technologies and systems) of UPS. Interaction between researchers and the CALMIP technical staff allows to optimize the return time of each calculation. For instance, the time needed to calculate the electronic structure near structural defects in a magnetite crystal has been shortened from 5h45min to 17 min.

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Simulations at the atomic scale in metallurgy

Certain mechanisms are difficult to test experimentally in metallurgy. The subject has greatly benefited from numerical simulations over the last 20 years, and the research performed at CIRIMAT is emblematic of recent progress in this domain.

Calculations and phase diagram predictions
Scientists are now able to describe the phase diagrams of various complex systems such as those containing just one atomic species as multi-phase systems (like ternaries). These ab initio simulations, based on quantum mechanics principles, provide data that can then be entered into thermodynamic equilibrium equations. Researchers can thus optimize many stable and meta-stable structures existing at equilibrium between phases.

The energies obtained are subsequently used at the same time as experimental data to optimize thermodynamic data bases destined for phase diagram simulations. These data bases can then be combined with diffusion coefficient data bases (such as those implemented in the DICTRA software, for example) in phase transformation calculations.

Defect migration
Another major worry for metallurgists is understanding the process of defect migration. Defect include vacancies, species in solution and extended defects. This information is very important for understanding how materials and structures age and is linked to experimental studies on degradation mechanisms or premature ageing (for example, by corrosion or hydrogen embrittlement). Nickel - a metal routinely studied by our group - is widely used in the aerospace and nuclear industries. Network vacancies in the metal are important for a number of mechanisms, such as corrosion, diffusion and cavity formation. At CIRIMAT, for example, researchers have calculated how such vacancies form and migrate. They have also observed that the energy of formation of 1.41 eV, and migration energy of 1.05 eV are in very good agreement with experimental data (1.46 to 1.72 eV and 0.97 to 1.04 eV, respectively).

Diffusion
CIRIMAT is also interested in interfaces, and in particular grain boundaries - where segregation, cracking and fast diffusion can occur. These systems are studied for just these reasons. For example, our simulations of niobium segregation in nickel grain boundaries suggest that it can easily concentrate at this interface. These results indicate that Nb atoms may change the mobility of the grain boundaries in the alloy and then influence its mechanical properties.

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Numerical simulations for understanding the behaviour of electrons in materials for spintronics

Spintronics has given rise to several industrial applications. However, the conception of new spintronic devices and an understanding of the fundamental physical principles that govern their behaviour requires high quality numerical simulations.

Spintronics is a relatively new research field in physics. The most important spintronic devices, namely spin valves and magnetic tunnel junctions, are made with thin magnetic metallic layers (the magnetic electrodes) separated by a thin non-magnetic spacer that has a thickness of a few nanometres. The electrical resistance of these multilayers depends on their magnetic configuration: it is smaller when the two electrodes have parallel rather than antiparallel directions.

Albert Fert and Peter Grunberg received the Nobel prize for physics in 2007 for discovering this magnetoresistance effect, which can be used to write and read a magnetic bit of information. This initial discovery has been followed by much fundamental and applied research based on the utilization of spin-polarized electric currents. The magnetoresistive properties of spin valves and magnetic tunnel junctions are used in the fields of magnetic memories and media - hard disk drive read heads or MRAM (Magnetic Random Access Memories) in computers use this effect.

Fundamental research

The physical phenomena that govern the electronic and magnetic properties of materials for spintronic applications are the subject of many fundamental studies. To understand the behaviour of electrons in these multilayers, we must use a quantum description of matter and numerical simulations must be performed in this framework. In general, these simulations use density functional theory (DFT), which allows to calculate the ground state density and energy of magnetic crystals. The basic equations that must be solved in this theory were proposed by Peter Hohenberg, Walter Kohn and Lu Sham in the 1960s. These are the basic equations of the codes used to calculate the electronic structure of crystalline materials. Solving these equations gives access to the total energy of the magnetic crystal, the density of states and the magnetic moment of the different atoms.

Tunnel current

Materials for spintronics have been studied for many years at CEMES by the Nanomaterials team. The numerical calculations and simulations performed allow for a better understanding of which electron states contribute to the tunnel current in magnetic tunnel junctions with Fe-based alloy magnetic electrodes (the physical properties depend on the electrode alloy composition for Fe1-xCox or Fe1-xVx electrodes), or with magnetite (Fe3O4) electrodes. Important magnetoresistive effects should be measured with magnetite electrodes, this material being half-metallic - that is, with metallic behaviour for spin-up electrons and with insulating behaviour for spin-down electrons.

Magnetic nanostructures

Recent research has also focused on tuning the magnetic anisotropy of multilayers with the aim of obtaining nanostructures with a magnetic anisotropy perpendicular to the thin magnetic layers. The systems with this magnetic configuration are very interesting: they can be used to record magnetic information with a very high density, and their magnetization can be switched using spin-polarized electric current with a relatively small intensity. The perpendicular anisotropy is actually due to the presence of interfaces between magnetic layers. In Ni/Co superlattices, the magnetization direction depends on the thickness of the successive Co and Ni layers (see figure). Another hot topic concerns the modification of the magnetic moments of metallic atoms near the interfaces of magnetic oxides.

Our numerical simulations are performed on the Hyperion supercomputer (CALMIP/UPS).
Theoretical study of the physical and chemical properties of carbon-based nanostructures

Thanks to their huge potential in terms of applications, graphene and carbon nanotubes are among the most exciting of nanomaterials.

Although the unique properties of graphene were theoretically predicted 60 years ago, the material (which is a single sheet of carbon atoms organized in a honeycomb lattice) was only isolated in experiments for the first time in 2004. This real breakthrough was acknowledged by the Nobel prize in Physics in 2010.

Graphene could be an ideal candidate for next-generation nanoelectronic devices, thanks to its amazing electron transport properties. Indeed electrons can whiz through the material at extremely high speeds.

Numerical simulations
Nanotubes, discovered at the beginning of the 1990s, are also emblematic systems in nanoscience. They can be thought of as rolled-up graphene sheets. Numerous fruitful experimental and theoretical studies, dealing with the chemical, mechanical, thermal and electronic properties of these materials have been performed over the last 20 years, with the development of sophisticated numerical simulations, and more particularly first-principles methods.

In this context, electronic-structure calculations, based on density functional theory, can be of great value. Thanks to the 1D or 2D character of these nanomaterials, calculations concerning just a few hundreds of atoms can be routinely performed now.

Electronic structure
A deeper understanding of the surface chemistry of such systems is one of the main objectives of the Physical and Chemical Modelling team at LPCNO, in conjunction with theoretical investigations of these electronic structures. In collaboration with experimentalists - led by Prof. Serp (LCC-ENSIACET), B. Lassagne (LPCNO) and P. Puech (CEMES), we are currently studying defect formation and stability, functionalization of sidewalls and metal-nanocarbon structure interactions. Indeed this interaction governs the behaviour of the growth of nanocatalysts based on metallic (Ru/Pt) atoms, the anchorage mode of a single magnetic nanoparticle on a carbon nanotube nanoresonator or even the catalytic activity of subnanometric clusters.

Supercells such as sulphuric acid are well known to be reversible p-dopants for nanotubes. Recent calculations have helped to interpret Raman spectroscopy results that suggest that the origin of the doping process is a non-covalent functionalization that induces a charge transfer between the tube and the acid.

Nitric Acid
Recently a combined experimental/theoretical study has led us to propose a reaction path, thanks to defect reactivity, that describes a fundamental step in the process of nanotube functionalization, that is, after the nitric acid treatment. Experimentally, this step is used to remove amorphous carbon, to oxidise the surface and yield carboxylic groups before complete destruction of the tubes.

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In 1900, the work of Paul Drude allowed to describe the phenomenon of electric current in a common metal such as aluminum by considering the motion of each electron independently and classically. However, soon after, the 1911 experiments by Kammerlingh Onnes in Leiden - and then the theory developed by Bardeen, Cooper and Schrieffer in 1957 - ushered in a revolution concerning the physics of metals. The latter theory explained how cooling a metal down to a temperature near absolute zero (-273°C) turns “normal” electric conductivity into “super”-conductivity. By contrast with the former, where the electrons scatter off the crystal lattice of the conductor and thus heat it up, the latter implies perfect conduction without any resistance to electric current, and thus no heating whatsoever! This seemingly magic effect can only be explained by quantum mechanics; in particular, the electrons tend to form pairs, which turns out to be key in the phenomenon of superconductivity. This effect begins at sufficiently low temperatures (-272ºC for aluminum), ordering the electrons into a collective state that allows them to move through a metal without experiencing any resistance.

The mystery deepens
A major surprise came in 1986, when Karl Müller and Johannes Bednorz discovered superconductivity in a new family of materials, based on copper and oxygen: the cuprates. These ceramics turn superconducting at the relatively “high” temperatures of about -150°C, where electron pairing is not expected at all! This is even more startling, given that at room temperature the cuprates conduct rather poorly.

What happens to these materials upon cooling? What mechanism pairs up the electrons and makes them superconductor? These questions, raised 25 years ago by materials now commonly called “strongly correlated”, still await an answer. Here, “strongly correlated” implies that charge carriers in these materials cannot be regarded as independent: it is the collective behaviour due to strong interparticle interactions, that gives rise to novel physics. Along with experiments carried out in laboratories across the world (such as the High Magnetic Field National Laboratory of Toulouse) understanding the physics at work in these “unconventional” superconductors represents a major challenge to theorists.

Novel quantum states
To solve these mysteries, the Strongly Correlated Fermion research team at the Theoretical Physics Laboratory (LPT) of the Institute for the Studies of Complex Atomic and Molecular Systems (IRSAMC) uses powerful analytic and numerical methods. Understanding and describing the collective behaviour of interacting quantum systems requires enormous computational power. With the help of supercomputers at LPT and at the computational meso-centre CALMIP, the researchers in our team use various cutting-edge methods. These involve the Lanczos algorithm that allows us to diagonalise giant matrices of many billion numbers, as well as the Quantum Monte Carlo method, whereby supercomputers simulate the dynamics of very large ensembles of interacting particles. The problem of strong correlations gives rise to a variety of new concepts from novel quantum states of matter to frustrated quantum magnetism and quantum entanglement. It is through pursuing these new ideas that novel theoretical methods develop, allowing us to step beyond established concepts. This year, we celebrate the centennial of the discovery of superconductivity, but the great adventure has only just begun!

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Uncovering the mystery of high-temperature superconductivity
Why do some materials superconduct when cooled down to “only” -150°C, rather than to temperatures near absolute zero (-273°C)? Research carried out at the Theoretical Physics Lab in Toulouse shows that these materials may host novel quantum states of matter.
Atomic-scale modelling for biohybrid molecules

Nanobiotechnology exploits biological and biohybrid molecules as structural materials and integrates them into nanodevices. The objective is to modify and control these complex systems provided by nature and couple them with technologically traditional materials (such as semiconductors, metals and oxides). These new developments should lead to a wide range of applications, notably in the fields of health and the environment.

Proteins can be considered as real molecular machines, with specific, sophisticated and adjustable functions. Nucleic acids also have unique self-assembly and hybridization properties that offer endless possibilities for nanopatterning, for instance. Although the idea of adapting these molecular objects to create new biohybrid devices has been considered for years, we are still far from using these structures in real-world applications. To be able to ensure the design and manufacture of DNA-based devices, it is crucial to understand molecular mechanisms at the atomic scale. This level of comprehension requires sophisticated numerical simulations. Today, modelling these biomolecules and integrating them into non-biological environments is our greatest challenge.

Multiscale simulation
At the LAAS-CNRS, in the nanoengineering team, we are developing models to predict both the structure and activity of biological and biohybrid molecules. We are especially interested in the way they may be affected by different modifications and a non-biological environment, as they are at the core of a nanodevice. To this end, we are developing innovative and dedicated tools, with the aim of integrating the materials into the larger context of multiscale simulations. To this end, we first designed the "Static Mode" method that allows us to compute the deformation of macromolecules induced by external excitations. The idea is to use this method directly to explore the intrinsic properties of biomolecules, but also to adapt it in a "docking" procedure - that is, to predict interactions with a view to assessing the impact of intermolecular interactions on partner structures and activity.

Bioinspired technologies
This approach can be used on "traditional" biological samples (particularly enzymes for pharmaceutical and medical applications: HIV protease, and DHFR). Pioneering work has also been performed in the field of bioinspired technologies in various fields of activity that include molecular motors (Ca²⁺ ATPase, myosin and chaperonin) and modified/functionalized DNA. These calculations accompany the LAAS experimental developments in DNA-based technologies, notably directed towards the development of aptamer sensors for medical diagnostics (cancer, for example) and the environment/health fields (water pollution).

The design of these devices raises many questions, such as how the environment influences aptamer folding, the choice of the detection device and its effect on the aptamer, the aptamer/target interaction mechanism, or the specificity of the sensor, to name but a few. To date, these issues are fundamental and generally applicable to all processes of bio/non-bio functional coupling.

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>>> Marie BRUT, UPS professor at the LAAS (CNRS lab associated to UPS).

>>> Structure of the dihydrofolate reductase (DHFR) catalytic site. Nicotinamide and pterin rings are shown, as well as the C4 and C6 atoms involved in hydrid transfer. We have shown that the δ2 methyl group allows to adjust the C4-C6 distance in a preferred direction and thus play a crucial role in catalysis.
Simulations at the atomic scale are crucial for the development of nanotechnologies and the elaboration of new materials. Three typical examples of such simulations, from the “matériaux cristallins sous contrainte” group at CEMES are presented herein.

While glass is fragile (it breaks), metals are easily deformed under an applied external stress. This ductility, the ability to be deformed without breaking, comes thanks to the presence, inside the material, of particular kinds of defects known as dislocations. Under an applied stress, the density of dislocations increases and they move, allowing the material to plastically deform. The study of dislocations and how they move is therefore crucial to understanding the plasticity of materials.

Among the different kinds of dislocations that exist, screw dislocations are particularly important in some metals like titanium, an important metal for the aeronautics industry. Their atomic structure cannot be determined experimentally and atomistic simulations are therefore used to study these structures using a quantum mechanics approach. Evidence for numerous metastable structures have been found and the results could explain how dislocations move in titanium and thus the plastic deformation behaviour in this metal.

They self-assemble...
Many other physicochemical phenomena have also been understood using atomistic modelling. Another example studied by the CEMES scientists is the self-assembly of some molecules when they are deposited on a substrate. Many applications are expected from the growth of organic molecules on crystalline substrates: elaboration of Organic Light Emitting Diodes (which would be very cheap to produce compared to existing technologies) or Organic Field Effect Transistors.

Due to their weak interactions, these molecules can self-assemble on a substrate. A precise knowledge of the molecule-molecule and molecule-substrate interactions is required to fully understand these self-assembling architectures, as well as their electronic and optical properties. For instance, phthalocyanines (Pc), a very well-known family of molecules used as dyes for solar energy conversion or for rewritable optical discs, can self-assemble in different ways. On a gold surface, they self-assemble parallel to the surface plane in a bidimensional lattice, whereas on the surface of salt (NaCl), they come together in a tridimensional structure. Using atomistic simulations (molecular mechanics), we have shown that the interaction Pc-gold is stronger than the interaction Pc-Pc, whereas it is the opposite in the case of the NaCl surface. This difference can explain the origin of the diverse self-assembling properties.

Acoustic waves
Similarly to the self-assembly of molecules, the self-organization of semiconductors and metallic nanostructures on a substrate surface is a promising approach for the electronics and optoelectronics industries. Indeed, such an approach would avoid the expensive and delicate process of lithography. The scientists in the group have also recently proposed a new elaboration technique that would potentially allow better control of self-organization at the nanoscale.
Six years later and taking the recent evolution of cancerology in Toulouse into account, we now review this scientific field again. Indeed many of the Toulouse teams specialized in cancerology now look set to benefit from the Oncopole (the next City -polis- of Cancer), whose clinical and scientific programme is now well defined.

Clinical trials
With respect to clinical and translational research, the Oncopole will be strongly involved in both haematological and gynaecological neoplasia. In particular, it will develop early clinical trials devoted to promote “first-in-human” tests of new molecules.

Regarding basic science, tumour microenvironment, tumour immunology and genome maintenance will be especially studied at the Oncopole.

Beside the teams that will work directly at the Langlade Oncopole, other research teams will also belong to the Toulouse Cancer cluster. All these teams will belong to the RTRS foundation and will bring complementary knowledge, such as gene expression, development and integrative biology, immunology and structural biology to the fore. Here we present the main strategies and last data to come out from the four Oncopole divisions - namely clinical and basic research, technological transfer and pharmaceutical R&D.

University hospital and research
Paul Sabatier University is the common denominator behind all the academic programs of the Oncopole: it is the “U” of the University Cancer Institute, which includes the next Cancer Hospital and its adjoining Cancer Research Centre (INSERM/UPS/CNRS) as well as the ITAV lab at the Pierre Potier Centre (University of Toulouse/CNRS). UPS is also moving forwards with the support of the Innabiosanté foundation, a national organisation. It also supports TOUCAN (Toulouse Cancer) Labex and SIRIC (Site de Recherche Intégré sur le Cancer) as well as the “museum of cancer medicine” at the Oncopole. Besides this key role as leading organizer, UPS will encourage the biotech companies to set up in the area by encouraging interdisciplinary programs at the Oncopole.

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Finding new therapeutic approaches: the great challenge of CRCT

Early diagnosis, gene therapy, treatments designed and tailored to cancer aggressiveness and to patient response. Anticancer approaches being studied in the Cancer Research Centre at Toulouse are more accurate, targeted and efficient.

The accumulation of genetic disorders explains why a healthy cell becomes a cancer cell. Identifying distorted cells in each cancer and finding new ways to fix these disorders are a major subject of research. As part of phase I/II clinical testing led by Toulouse Hospital, Louis Buscail’s team is testing gene therapy in pancreatic cancer and hepatocellular carcinoma.

Aggressiveness matters
Cancer aggressiveness depends on the microenvironment, meaning that tumour development is linked to its surrounding healthy tissue. One of the major lines of research in CRCT is the study of this tumour microenvironment. Recently, new markers that determine the aggressiveness of pancreatic and lung cancers have been discovered.

The CRCT teams are also interested in the resistance of cancer cells to chemotherapy and induced relapse. The aim of this work is to increase the duration of remission and improve the quality of life for patients. The research particularly targets blood cancer (leukemia, lymphoma and myeloma) and focuses on acute myeloid leukemia and lymphoma as real hope exists in improving treatments for such pathologies.

The efficacy of treatments may vary
The efficacy of treatments is different from one patient to another. In order to improve the efficacy of current treatments and, obviously, to propose better ones, several CRCT teams are focusing on the reasons for such differences. These new therapeutic options are still at an experimental stage and will be developed at the Institut Universitaire du Cancer (IUC) in collaboration with the CRCT teams.

We share a “bench to bedside” approach, meaning that our aim is to adapt our fundamental research to specific clinical problems in patients. From the genome of a small sample of malignant cells, we should be able, in the short term, to identify abnormalities involved in patient cancer. Then, clinicians from the IUC will be able to treat such personalized information in order to offer the patient the best therapeutic options.

“A la carte” treatment
Due to the personalization of medicine, the emergence of new technologies in early diagnosis and the development of low-cost sequencing of the human genome, the panorama of oncology is growing larger each day. Whereas the upcoming challenges in cancer research will be scientific, medical and technological, some challenges also need to be faced in the sociological, ethical and economics fields. To rise to these challenges, mathematicians, physicians, specialists in IT, in social sciences and in the economy will join the CRCT teams to develop various research projects. Consequently, the research topics and fields developed at the CRCT in the coming years will be multidisciplinary – a major vocation of our research center.

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The ITAV teams (led by B. DUCOMMUN and C. VIEU) focus on the development of new models of 3D cell culture, engineering of microdevices and the implementation of new imaging tools to study tumour proliferation and assess response to treatment. A major achievement in the laboratory has been the development of a new cell imaging system, called SPIM, to visualize three-dimensional biological structures and large organizations under the conditions that allowed their development.

A “SPIM routine” is now open to the scientific community and available on the ITAV imaging core facility at the Genotoul and certified IBiSA*. This achievement and the pursuit of original developments in imaging are based on collaborations with teams from IRIT and IMT.

To study tumour proliferation, the teams are also focusing on original models of spheroids, a 3D model closer to tumours than monolayer cell cultures, mimicking their organization in vitro. Development of devices to control growth can be used to study the effect of mechanical stress on tumour development. SPIM microscopy also allows in-depth imaging of the spatio-temporal aspects of the dynamics of cell proliferation in 3D spheroids as shown in the figure. These cell models, engineering original devices, and the development of imaging tools open the way to the study of how 3D structures respond to chemotherapeutic agents and ionizing radiation.

* The development of this new instrument would not have been possible without the financial support of the following institutions and charities: CNRS, Université Paul Sabatier Toulouse 3, Région Midi-Pyrénées, MRCT, fondation InVivoSanté, Cancéropôle Grand-sud Ouest, GIS IBiSA, Ligue contre le Cancer, Association pour la Recherche sur le Cancer.

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The Institut Universitaire du Cancer (IUC) will focus on fundamental and clinical research, and its aim is to provide “bench-to-bedside” solutions to patients. Its main goal is to offer patients the latest in cancer treatment. Wards will be dedicated to research and associated with 13 platforms on the same site that take advantage of the latest technology in cancerology, together with the Toulouse Centre of Research in Cancerology (a joint Inserm/UPS/CNRS research unit). Finally, a biology resource centre in oncology – one of a kind in the midi-Pyrénées region – will be put in place on the IUC site too.

Improving patient care
To speed up initial patient care, a specialised multi-task consultation platform will be created. To ensure that all cancer patients in the region have equal access to care, the IUC will organise a therapeutic decision-making and patient-guide centre. This centre will bring together public health care organisations. A special exchange and teaching centre for health professionals will also be set up. The IUC is a great opportunity to restructure and rationalise public health care in oncology for the Toulouse region. Three establishments in the area (the IUC, Rangueil-Larrey and Purpan) will thus be specialised in oncology. The IUC itself specialises in haematology, female oncology, ear, nose and throat (ORL) cancers, melanomas, sarcomas (rare but very aggressive and resistant tumours) and urology. Other cancers will continue to be treated at the Purpan and Larrey-Rangueil hospitals. Moreover, the IUC will be home to a certain number of highly specialised infrastructures that will be shared with these hospitals and partner establishments in the region, such as intensive care, specialised radiotherapy and research centres.

Screening
At present, screening is in place for a certain number of cancers. However, once performed, the patient is often left to his own devices for the follow-up medical. The IUC hopes to remedy this by co-coordinating the organization of patient care and creating a special centre dedicated to screening follow-up if anomalies are found during the initial procedure. This organization will allow the epidemiological study of early-stage cancers and their detection.

Michel Attal, professor at the university hospital, head of the haematology department at the CHU of Purpan, president of the Groupement de copération sanitaire de préfiguration at the IUC.

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A new public-private partnership to discover novel anticancer agents.

For more than 20 years now, the CNRS and the Pierre Fabre Laboratories have been developing common research programs aimed at discovering new anti-tumour agents. This partnership has been very successful and two alkaloids of the Vinca rosea are now being commercialized as anti-tumour drugs: Navelbine® (vinorelbine), used for the treatment of lung and breast cancer, and Javelor® (vinflunine), recently registered in Europe for the treatment of advanced or metastatic transitional cell carcinoma of the urothelial tract.

In January 2011, the Institut de Recherche Pierre Fabre (IRPF) and the CNRS founded a new joint laboratory, the Unité de Service et de Recherche (USR n°3388) entitled “Epigenetic Targeting of Cancer” (ETaC), which brings together basic and applied research.

The USR ETaC is based on three functional and complementary departments: two technological platforms dedicated to the chemistry of bioactive natural products (plant and microbial biodiversity, extractive and analytical chemistry, semi-synthesis and organic synthesis) and to pharmacological screening. The latter is a national screening platform. It received the IBiSA label in 2009 and plays a key role in the “Plateforme Intégrée de Criblage de Toulouse” (PICT) - miniaturization and robotization and chemical screening.

The USR ETaC is composed of a third team of chemists and biologists dedicated to the epigenetic regulation of cancer. Chemists and biologists work together to study the role and control of the epigenetics markers in cancer, in particular in metastatic melanoma, in close collaboration with the teams from Pierre Fabre Oncology Research.

The Laboratory works on basic topics (new targets and new molecular mechanisms) while keeping an eye on applications (candidate drugs).

Molecular and cellular level studies will bring a better understanding of epigenetic regulation, in particular DNA methylation, which is essential in tumorigenesis and in certain chemoresistance. The design of pharmacological and chemical tools (such as new DNA methylation inhibitors) will also allow us to understand the biological processes that are found in cancer, to propose new therapeutic targets and to discover new anti-tumour agents.

Towards clinics
The USR ETaC is based at the Oncopole of Toulouse in the new Pierre Fabre Research and Development Centre (CRDPF). As a joint unit, it collaborates extensively with other partner laboratories. The Oncopole (CRDPF, Centre Pierre Potier ITAV and soon the Institut Universitaire du Cancer and the Centre de Recherche en Cancérologie de Toulouse) will develop new innovative and collaborative projects that will go from basic research to the patient (“from bench to bedside”) through technology and pharmaceutical development.

The USR ETaC is very active in local scientific life too (it is member of the Institut de Chimie de Toulouse) and at the national and international level through many collaborations.

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Research at Paul Sabatier University

Research at Paul Sabatier University is spread across 62 laboratories, most of which are joint labs with the CNRS, INSERM, IRD, INRA and CNES.

2550 researchers and assistant professors, and 1200 technical and administrative staff work in these laboratories.

1600 PhD students are enrolled at UPS, in 11 doctoral schools of which 6 are run by UPS.

The four main poles of research are:

- **MST2I** (Mathematics and Science and Information and Engineering Technology): 9 labs and 5 federations
- **UPEE**: (the Universe, Planet, Space and Environment):
  - 7 labs, 1 observatory
- **SM** (Materials Science): 12 labs and 2 federations
- **SV** (Life Sciences): 26 labs and 5 federations

To these four major poles, add the **CIGEDIL** (Communication, Information, Management and Languages Didactics):

- 3 labs and one federation