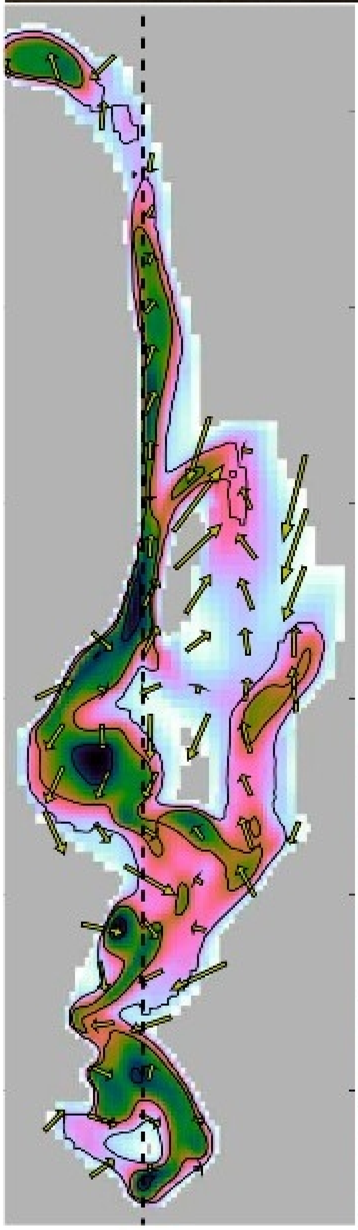
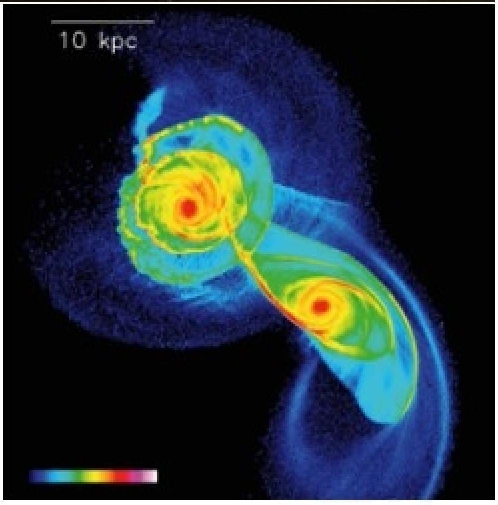
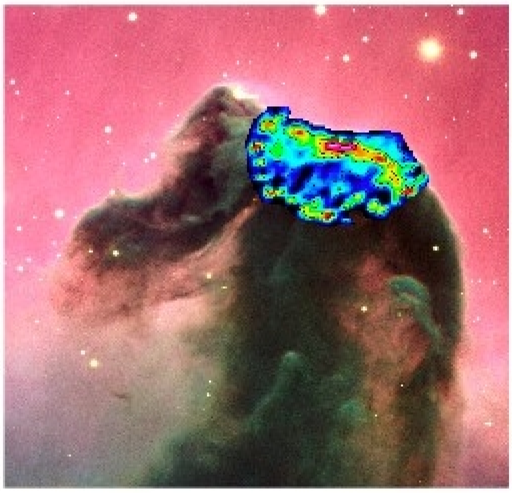
LABORATOIRE D'ETUDES DU RAYONNEMENT ET DE LA MATIÈRE EN ASTROPHYSIQUE ET ATMOSPHERES

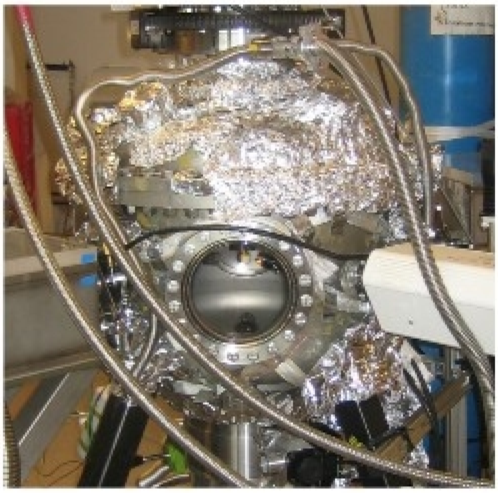


# LERMA²
# Project 2014-2018




## Vol.1 Scientific Project (version 2.2)





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Unité Mixte de Recherche 8112 - Contractualisation Vague D

The Atacama Large Millimeter Array (ALMA) under moonlight
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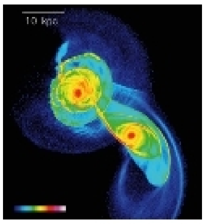
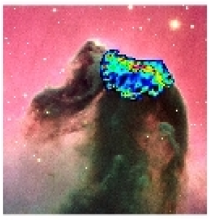



High-resolution enhancement of GALMER, the largest VO library of galaxy merger simulations
© Di Matteo, Combes, Semelin *in* La Recherche n°457, p. 28, Nov 2011

The experimental set-up SPICES for the study of surface photoprocesses of interstellar ICES analogues irradiated by vacuum-UV photons



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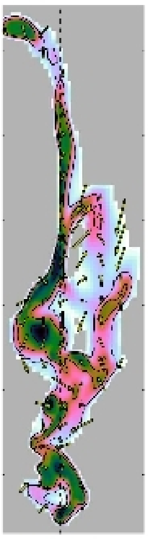

3D MHD simulation of turbulent interstellar cloud used for UV-irradiation calculations and synthetic spectra
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*Conception graphique S. Cabrit*

*Foreword*

The present version 2.2 of the LERMA project describes the program envisaged for the merged Unités Mixtes de Recherche 8112 (LERMA) and 7092 (LPMAA) for the period 2014 to 2018, reinforced with members of the ISM team of LUTh.

The structure of the document derives from the AERES requirements as expressed in their document S2-1-4-UR-Projet.pdf, for the 2012-2013 evaluation campaign.

It has been prepared by a small coordination group (S. Cabrit, F. Combes, M.-L. Dubernet, J.-H. Fillion, C. Prigent, M. Wiedner, V. Audon), with the much valued help of many colleagues, who took significant amounts of their time in order to prepare the various inputs to this project. Special thanks go to V. Bigot, F. Dayou, M.-L. Dubernet, F. Dulieu, E. Falgarone, M. Gerin, L. Girot, C. Janssen, P. Jeseck, J.-M. Krieg,, F. Le Petit, A. Maestrini, L. Pagani, B. Sémelin, C. Stehlé, D. Valls-Gabaud, C.-M. Zwölf, who have put much enthusiasm in conducting our two laboratories all along the preparation of this shared project, in a very constructive way.

This document has been formally approved by the Councils of LERMA and LPMAA on January 9$^{th}$, 2013

Michel Pérault, directeur du LERMA October 15$^{th}$ 2012 in Paris

(updated January 10$^{th}$, 2013)

## Structure of the document

# Volume I.

# Scientific Project

*Foreword*

Following the AERES guidelines given in document S2-1-4-UR-Projet.pdf, this document (Volume 1 of the Project documentation) contains 3 sections. The first section is dedicated to the presentation of the future laboratory, from an historical and institutional point of view. The second section presents the main objectives of the LERMA² project, and its national and international positioning, as it emerges from the constituting entities reports of the past period. The third section describes how the scientific project will be implemented, along with the methods and resources which will be needed and used.

The presentation of the scientific project follows the scientific organisation that has been put in place for the LERMA² project, in four thematic poles, which conduct all research projects of the laboratory. The thematic poles are numbered from 1 to 4 for simplicity :

1. Galaxies and Cosmology,
2. Dynamics of the ISM and Stellar Plasmas,
3. Molecules in the Universe,
4. Instrumentation and Remote Sensing.

As a consequence four separate sections of this document explain the major objectives and positioning of each of the four thematic poles.

The thematic poles are complemented by one common Scientific Services Pole, which organises the involvement of the laboratory in additional missions of the Laboratory, which are not research projects, but rely on our research potential. All of the activity is backed by a shared Technology and Research Support Pole. These components are instrumental to the project. As they are shared components, their presentation is obviously common to the whole laboratory.

# Table of Contents of Volume I

# Part 1. Presentation of the future Laboratory

# 1. Historical perspective

LERMA is rooted in the early development of radioastronomy, on one hand, and atomic and molecular physics applied to astronomy, on the other hand. Created in 2002 with the merging of the *Laboratoire de Radioastronomie Millimétrique* and of the *Laboratoire Atomes et Molécules en Astrophysique*, LERMA has grown to a mature research institute, fundamentally dedicated to molecular astrophysics and to the development and exploitation of powerful instruments for spectroscopic and spectropolarimetric imaging.

These fundamentals have triggered active investigations of the dynamics of stellar systems and galaxies, with more and more emphasis on galaxy, star and planetary system formation. Needless to say, these investigations have developed far beyond radio observations, into various parts of the electromagnetic spectrum, into numerical simulations and more recently into laboratory astrophysics. These developments resulted into a great diversity of activities within LERMA and into a very large network of collaborations and partnerships in France and abroad.

The other main constituting piece of the future LERMA² laboratory is the laboratory known today as LPMAA, *Laboratoire de Physique Moléculaire pour l'Atmosphère et l'Astrophysique*, once *Laboratoire de Physique Moléculaire et Applications*, itself an evolution in the early 90's of the former *Laboratoire de Spectroscopie, then de Spectronomie Moléculaire*, which stemmed from the 50's and early 60's *Laboratoire de Chimie Physique de la Faculté des Sciences de Paris*, where molecular lasers were first developed, along with high resolution spectrometry. LPMAA nowadays is a fundamental physics laboratory dedicated to modern molecular physics, and also committed to applications in various areas, mostly astrophysics, atmospheric physics and environment.

Finally a very active research team with profound expertise in fundamental molecular physics, and in astrochemistry has also decided to join the LERMA² project. This team, presently part of the *Laboratoire Univers et ses Théories*, has had close collaborations with LERMA for decades, and its coming closer to LERMA is an expected and welcome move.

As a consequence of these diverse and very complementary origins, the new laboratory proposed here brings a wealth of expertise together in a single operational structure

An heritage from the early developments of the two historical components of LERMA is the implantation of the lab within 4 institutions, 3 of them are venerable institutions in Paris, namely the Sorbonne (UPMC), the Observatoire de Paris (OP), and the École normale supérieure (ENS). The 4th institution, on the other hand, is a recently created University in the Paris area, at Cergy-Pontoise (UCP). LPMAA has been a UPMC laboratory since ever.

The resulting geographic dispersion of the research teams over the Paris area much influences our laboratory life. The advantages and drawbacks of this situation have been addressed in the LERMA report. The widely shared belief that the scientific advantage of the combination of these components overrides the drawbacks determined the proposed organisation of the new laboratory in 4 research thematic poles, which happily traverse geographic boundaries. As they stand today, these 4 poles arose from intense internal discussions which started during the March 2011 *Journées du LERMA*, when the whole lab convened at a secluded residence in Sologne, and continued throughout the following year where the future of the lab was very seriously considered.

# 2. Characterisation of the activity

The primary mission of LERMA is fundamental research in astrophysics. Created as research unit in astrophysics, focused on the development and exploitation of short wavelength radio-telescopes, the multidisciplinary practice which developed from the needs of fundamental parameters in molecular physics, and from the needs of new instrument concepts, and of components of ever growing sensitivity, also expanded it into a laboratory of fundamental physics and applied technology. The new capacities in turn triggered the development of new applications for the instruments developed, especially for Earth and planets observations. The progress made in fundamental astrophysics, on the other hand, attracted scientists who developed different methodologies, including observations over most of the electromagnetic spectrum, and laboratory experiments at high energy densities.

The primary mission of LPMAA is fundamental research in physics. It also quickly developed applications to atmospheric physics, and later on to astrophysics and environment research. Coming from a different horizon, its tracks became very close to some of those followed by LERMA, to the point where merging both laboratory projects appeared as a very reasonable goal, leading to stimulating new synergies.

As a consequence the new laboratory is dedicated to fundamental research in astrophysics and in physics, with the ambition to constantly increase our level of understanding of natural dynamics, from the nanometre size scale of molecules up to the largest astrophysical scales. Among the thematics studied by the LERMA² teams, are some of the main puzzles of modern astronomy, such as the formation of new stars, the cycle between diffuse and dense gas, star formation, and enrichment in heavy elements in the interstellar medium, dynamics and formation of galaxies in a cosmological context, the nature of dark matter, and the origin of structures.

As secondary missions, we can quote the promotion of novel instrumentation concepts and technology, the development of applications of these progresses to adjacent fields of fundamental or applied research, and the dissemination of the new knowledges and know-hows through education, academic and economic partnerships, as well as outreach in the broadest sense.

Although environmental challenges are not primarily in our roadmap, we would feel irresponsible if not offering the expertise and technology that we have developed in a very different context, whether fundamental physics or astrophysics, to applications which may have a significant impact for the solution of major contemporary issues. Spectroscopy, sub-millimetre instrumentation and high performance simulation and data processing may be significant assets for our contemporary world, which we cannot keep for fundamental research only.

# 3. Organisation chart and regulations

## 3.1. Organisation of the future LERMA²

### 3.1.1. The Poles

The Laboratory is organised as 4 *Thematic Research Poles*, 1 *Technology and Research Support Pole*, and 1 *Scientific Services Pole*. Each Pole has a coordinator and an internal organisation adapted to its activities. The coordinator of each Pole drives the scientific policy of the Pole, keeps the Pole members informed of the Lab's internal life and represents the Pole in its entirety within the Executive Committee.

#### a) Thematic Poles

The 4 thematic poles of the LERMA² project are:

1. Galaxies and Cosmology
2. Dynamics of the Interstellar Medium (ISM) and Stellar Plasmas
3. Molecules in the Universe
4. Instrumentation and Remote Sensing.

This simple scientific partition resulted from the collective work started in 2011 within LERMA in preparation of the future, and closely involving the Laboratoire de Physique Moléculaire pour l'Atmosphère et l'Astrophysique (LPMAA), and later the members of the Interstellar Medium team of Laboratoire Univers et ses Théories (LUTh) willing to join the LERMA² project.

#### b) Technological and Research Support Pole

All administrative and technical staff members are attached to the Technological and Research Support Pole (in short: Support Pole). Given the high level of expertise required to carry out their work, most of them also belong to one of the Thematic Poles, as primary or secondary affiliation. This shared structure has been progressively installed after the nomination of the LERMA technical director, in charge of the technical section of the Pole, in order to facilitate exchanges among specialists of similar fields, to optimize the workload of our administrative and technical staff, and to improve their career perspectives. The resulting links, which developed across our many boundaries, play a constructive role in our lab development. This Pole is further described in the implementation chapter of the document.

#### c) Scientific Services Pole

Non research scientific activities relying on or deriving from our main research mission will be grouped in this transverse structure, which is used to coordinate, where and when needed, the lab members involvement in the national *Services d'Observation*, teaching and training activities, outreach and communication.

### 3.1.2. The Sites

The Laboratory is hosted in various sites by its governing institutions: *Université de Cergy-Pontoise*, *Ecole Normale Supérieure*, *Université Pierre et Marie Curie*, and *Observatoire de Paris*. The latter premises are split on one site in Paris and one site in Meudon. Each site has a person in charge, the Site Manager, whose role is to facilitate the daily life of the site. The Site Manager supervises the site operations in the fields of finance, human resources and premises. He/she represents their site within the Executive Committee, and relays the information between the Director and the personnel hosted on the site. He/she also actively represents the Director within their hosting Institution. The site manager may also be formally nominated as Deputy Director of the Laboratory (the deputy director's duties will be defined by the Internal Rules and Regulations Document, which still needs to be written down, as explained below).

### 3.1.3. The Executive Committee

The Executive Committee (*Conseil de Direction* = CD) is composed of the Direction Team (director and deputies, technical director and administrative manager(s)), the Pole coordinators, and the Site managers. The CD is the place where the activities of the Poles are presented in relation to its resource needs, and where the laboratory policy is formulated with respect to budget, staff recruiting, premises, and other priorities impacting the laboratory's development and its scientific strategy. The CD is also the place where all useful informations are shared, with the obligation for the Pole coordinators and Site managers to relay the relevant information from and to the Poles and Sites. As a consequence each meeting of the CD is preceded and followed by Site and Pole internal consultations led by the person in charge.

The CD, restricted to the Direction Team and persons in charge of the annual professional interviews with the technical personnel (ITA/IATOS), who may be invited for this purpose if not members of the CD, debate and rank the Laboratory staff applications for promotions, after the end of the annual interviews. Feedback to the personnel is given by the persons in charge of the interviews.

The executive committee meets on average once a month.

### 3.1.4. The Advisory Council

The Advisory Council, or Laboratory Council (*Conseil de Laboratoire* = CL) is composed of a majority of elected members, and is chaired by the Director. The following strategic decisions prepared by the CD are presented by the Director to the Council for approval: recruiting and budgetary priorities, ranking of PhD proposals, when not financed from specific contracts, and ranking of proposals to announcements of opportunity, when requested, and only if the schedule makes it possible.

The CL establishes specialised committees in charge of leading the Laboratory's reflection on selected topics, like premises, careers, etc... The role of the CL will be detailed in the future Internal Rules and Regulations document (*Règlement Intérieur*).

The LERMA² Council meets 3 to 4 times a year. As a tentative agenda:

- the winter meeting is dedicated to the budget,
- the spring meeting addresses institutional policy, permanent staffing priorities, and

PhD students recruitment,

- the summer meeting reviews the progress made on the main LERMA² projects, and the workload of the technological and research support Pole,
- the fall meeting prepares for the next run of applications to the regional, national and European calls for proposals.

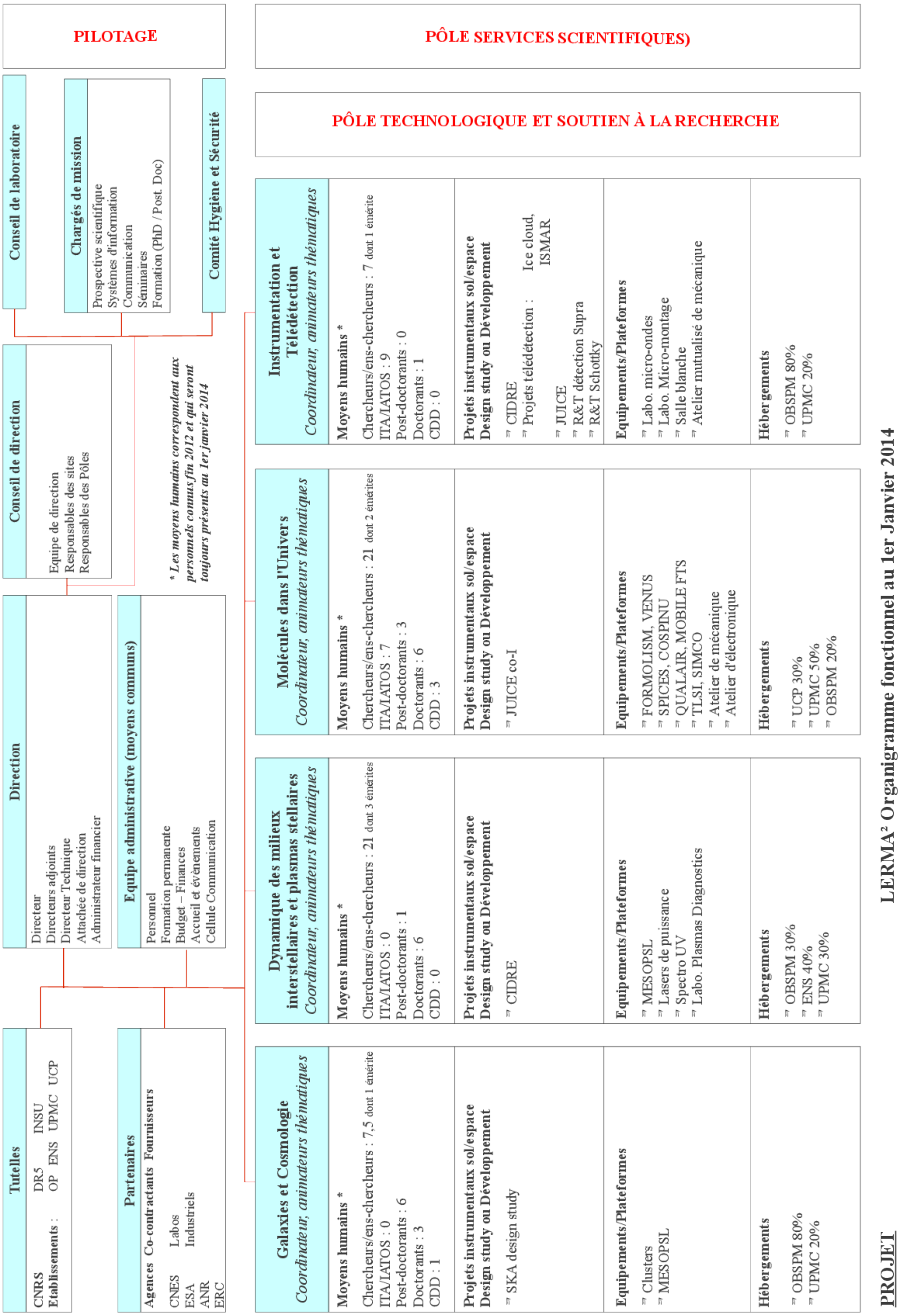


*Fig. 3.1: Functional chart of LERMA²*

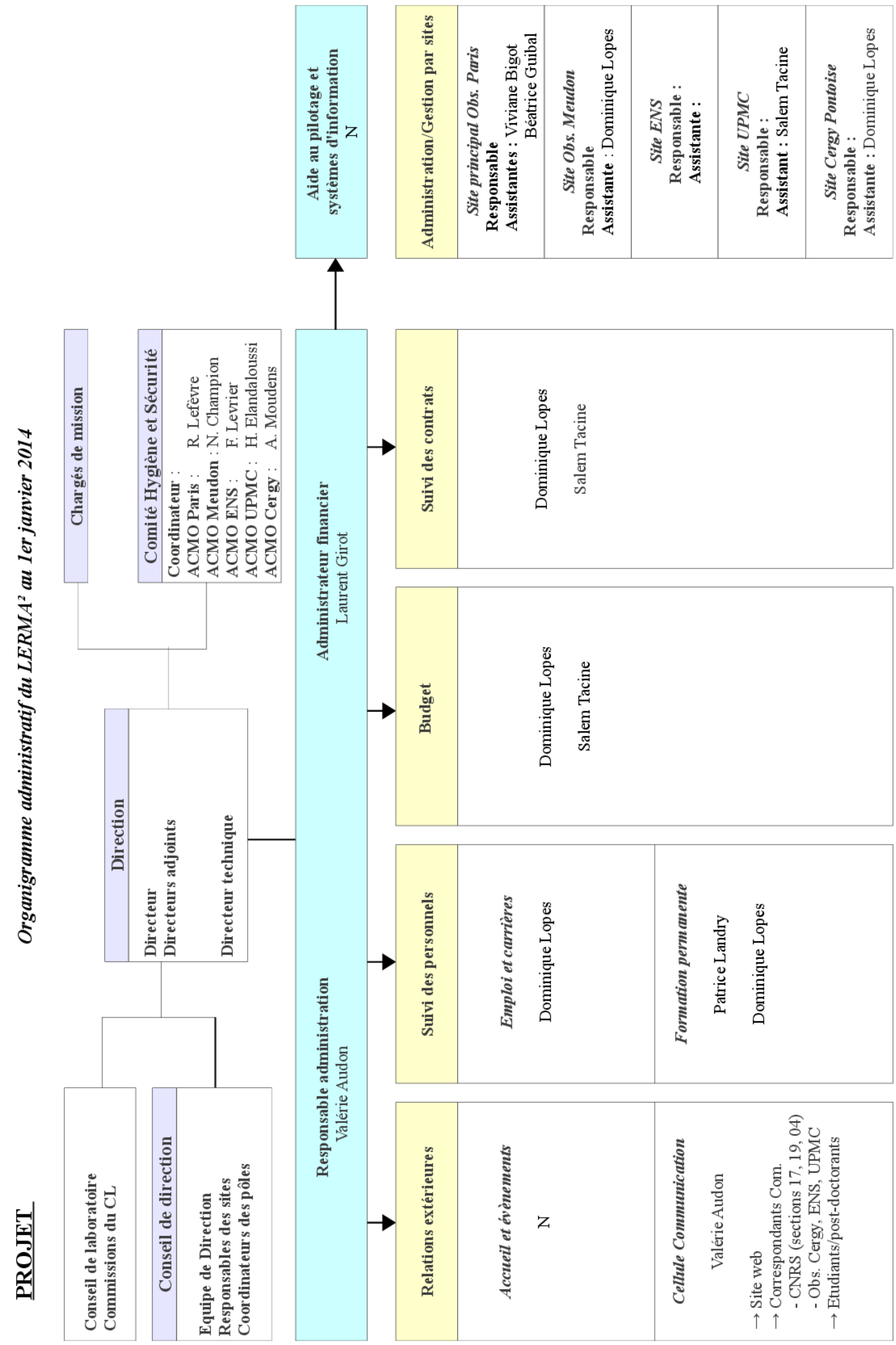


*Fig. 3.2: Administrative chart of LERMA²*

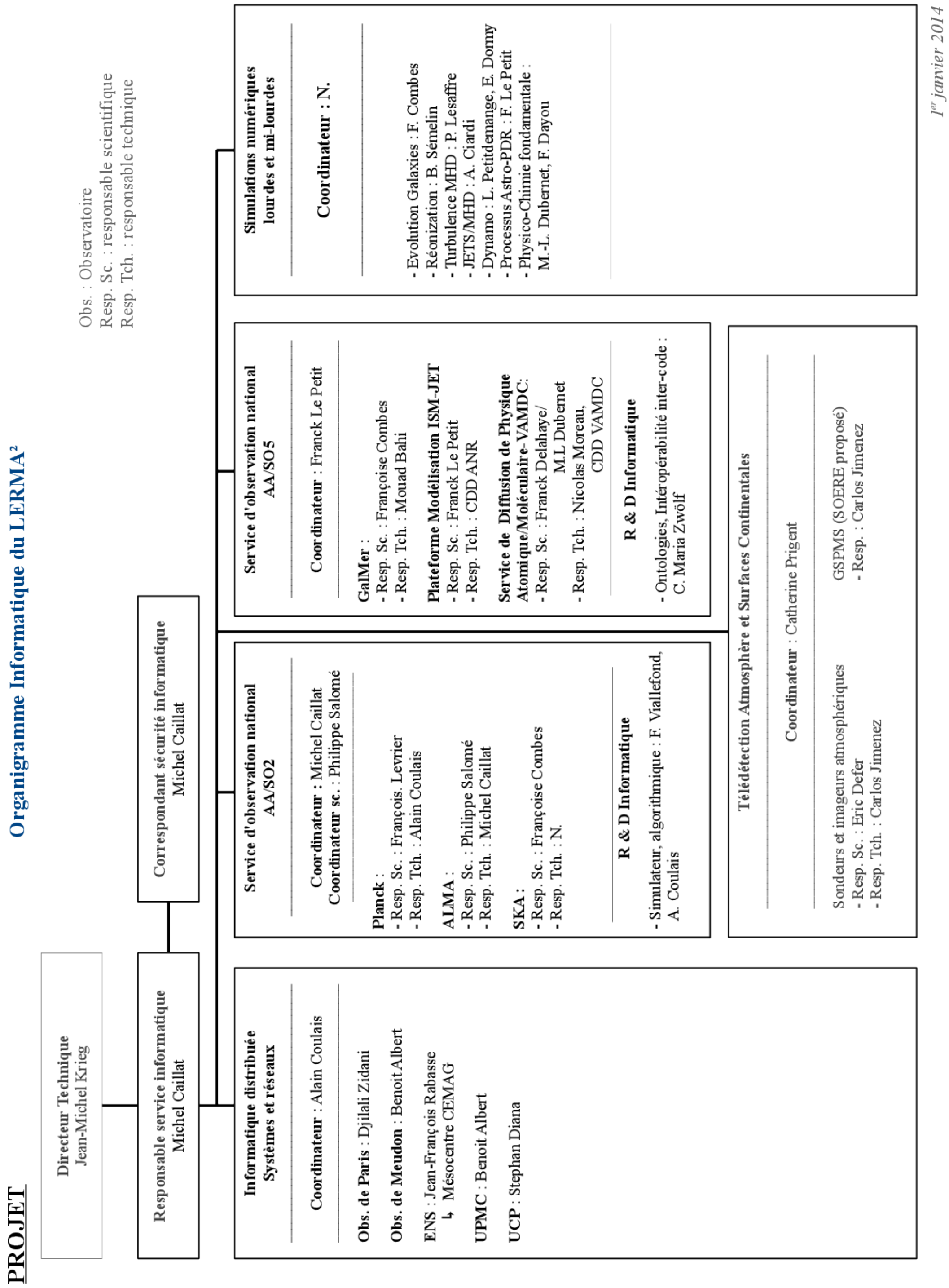


*Fig. 3.3: Computing and information systems activities of LERMA²*

## 3.2. Internal regulations

### 3.2.1. Internal Rules and Regulations Document

The Internal Rules and Regulations (*Règlement Intérieur*) of a *Unité Mixte de Recherche* (UMR) derives from generic texts prepared by CNRS and agreed with all governing institutions of the Laboratory. The model regulation text for an UMR can be found at url: `https://upload.obspm.fr/get?k=tX6ElEWvVk4gbzU2ou0`.

The Observatory obeys its own statutes established by decree 85-715 `http://presidence.obspm.fr/archives/decret85-715.pdf`. This decree defines the research missions to be carried out in *Départements scientifiques*.. For obvious reasons of simplicity the Observatory had decided to identify *Départements scientifiques* with the UMRs, without worrying for the few incompatibilities between the 2 sets of rules. The corresponding document can be read at url: https://upload.obspm.fr/get?k=iLS16zitJV4T7AaAfsM.

These incompatibilities essentially boil down to a *Département* being administrated by its elected Council, which elects the director, while for a UMR the elected/nominated Council is an advisory body to the director, himself nominated by the governing institutions.

The Observatory laboratories have been functioning for many years in a CNRS complying spirit, without caring for this inconsistency. The inconsistency was pointed at by CNRS in 2010 however, which invalidated the internal regulatory document. LERMA thus presently needs to revise its internal regulation text.

In addition, for independent reasons, the Ministry requested the Observatory to rewrite their own internal regulatory document, which implies that the functioning of its components currently relies on open foundations.

The merging of LERMA with LPMAA is a good opportunity to write new regulatory documents. Year 2013 will be the right time to do so, provided the Observatory issues its own new regulations, and a suitable agreement between all institutions is found, in agreement with the principles enforced by CNRS. Because this work is not done yet, we can only announce that a committee will be set up for this purpose in 2013 in order to define the *Règlement Intérieur* of LERMA[2].

### 3.2.2. Health and Safety

We intend to harmonise our Health and Safety procedures among all our sites :

Each site (Observatoire de Paris Meudon and Port-Royal sites, ENS Lhomond site, UPMC Jussieu site, and UCP Neuville site) has its own *agent de prévention*. Two meetings will be organised each year (one to write the *document unique* and the second one 6 months later to check the actions performed).

A guide book of lab security will be written for newly-appointed personnel, in complement to existing security guides of the hosting institutions.

We will organise common H&S training sessions and centralise the bookkeeping of H&S training.

According to the new decree 2010-750 for artificial optical sources use, the requested security improvements will be set up for all sites. Individual sites issues are addressed in the relevant *Health and* Safety reference document of the UMR, for each site, updated yearly.

### 3.2.3. Information System

The person in charge of the IT security issues for the UMR receives all related documents, and redistributes the relevant information to all affected agents, and supervises the implementation by the IT personnel of the security recommendations across all sites of the laboratory. The person in charge is the laboratory's point of contact on these questions with the IT Security officers of CNRS and of our hosting institutions.

### 3.2.4. Intellectual Property

LERMA² relies on the dedicated services on contractual activities and legal matters of CNRS and of our hosting institutions. Common agreements are found on a reasonable case by case basis on the relative rights and duties of the different partner institutions (hosting the project, providing administrative and financial support, and/or employing the personnel) and of the individual actors, based on rules commonly agreed in the quinquennial contract of the laboratory.

# Part 2. Positioning and Scientific Objectives

# 1. SWOT analysis of LERMA²

## 1.1. Strengths

### 1.1.1. End-to-end study of the dynamical cycle of cosmic matter

LERMA² is one of the few astrophysics laboratory in the world studying the dynamical cycle of cosmic matter over its full range of temporal and physical scales, from the early fluctuations encoded in the cosmic background signal, through the phase of galaxy growth and re-ionisation, to the condensation of molecular clouds into stars and planets, and down to the atomic, molecular, and grain processes that determine the gas temperature, composition, and emergent spectra. A common characteristic of the LERMA² approach of these problems is not only to observe (particularly but not exclusively in sub-mm spectral lines), but also to develop self-consistent physical models in order to interpret observations and thus gain a deeper understanding of the origin and fate of all cosmic structures. Underlying all of these modelling efforts, and common to all scales, are the fundamental issues of instabilities, dissipative gas dynamics, feedback (from stars or AGNs), matter-radiation-magnetic field (de)coupling, and their chemical/spectral signatures. This common thread is a strong asset for our laboratory, as it naturally creates a common language and shared interests among its members, who can then benefit from relevant ideas or methods developed outside their area of expertise. An example of such cross-scale synergies is the use of magnetized molecular cloud simulations by LERMA² members to model (and eventually remove) the large-scale galactic foreground signals in the *Planck* survey of the cosmic background.

### 1.1.2. Cutting-edge expertise and international recognition in all 4 scientific poles

All 4 thematic poles of LERMA² have developed cutting-edge expertise reaching the highest international standards in their respective areas. Examples include: Simulations of galaxy formation and dynamics, and of the re-ionisation signal in HI (Pole 1); MHD-modelling and chemical diagnostics of the dynamics of interstellar and stellar plasmas (Pole 2); molecular collision calculations and ultra-vacuum experiments of gas-ice and photon-ice interactions (Pole 3); design of efficient THz multiplier and mixer devices, and powerful inversion tools for multi-spectral remote sensing (Pole 4).

This high level is testified by the leadership of LERMA² researchers in numerous large international collaborations (PI of major observing projects on e.g. *Herschel,* IRAM, VLT, ALMA, (co)PI or science coordination of European networks such as JETSET, VAMDC and of world-wide consortia such as the Opacity Project). Another testimony of international recognition is the large number of nominations of LERMA² researchers in international science teams (eg. *Planck* core team), program committees of major facilities, review panels, and visiting committees of major international institutions; as well as their numerous invitations to international conferences and schools, co-supervision of foreign Ph.D. students, and foreign senior scientists visiting each year for at least 1 month (cf. LERMA and LPMAA "Results" documents for more details).

### 1.1.3. Multi-method approach

Another key strength of LERMA² is the simultaneous presence of observers, theoreticians, numericists, experimentalists, and instrumentalists. While these expertises are now found in many laboratories, the numerous collaborations built over the years in LERMA and LPMAA make the interactions particularly tight. This allows us to tackle each problem from a variety of angles and, building upon these complementary approaches, to shorten the path between data and discoveries. For example: Theoretical and experimental studies of atoms and molecules in Poles 2 and 3 are adapted "in real time" to address new issues raised by observations (eg. chemical anomalies in molecular clouds and stellar spectra, formation of species on grains, effect of irradiation…), and vice-versa; intensive numerical HD and MHD simulations and laboratory plasma experiments are used to rapidly test and improve theoretical ideas, and to predict the best observational diagnostics (Poles 1 and 2); instrumental research in detector technology and advanced multi-spectral inversion methods (Pole 4) lead to the development of new observational opportunities (eg. HIFI/*Herschel*, CIDRE and SWI projects). These many capabilities working together on a transverse problem are a formidable underlying potential to produce significant breakthroughs.

### 1.1.4. Strong link with Physics and involvement in teaching

A rare characteristic of LERMA$^2$, among astrophysical laboratories depending primarily from the "Universe Science" Institute of CNRS, is its strong interface with Physics. The deeply rooted interest of LERMA$^2$ in physical processes is especially obvious and vital for our research activities in eg. primordial universe (Pole 1), MHD turbulence/transport and the emerging domain of Laboratory Plasma Astrophysics (Pole 2), fundamental molecular physics (Pole 3), and detectors (Pole 4). This multi-disciplinary aspect is a major strength of our laboratory, as we believe (and have verified) that a deep understanding of physical processes and non-linear phenomena is essential to major discoveries in the study of the cosmic matter cycle. Our secondary university partners (ENS, UPMC, UCP) all host strong Physics departments that provide an optimal environment to sustain these links, through direct collaborations and teaching activities. Currently, two thirds of LERMA² scientists have teaching duties. Their courses cover Fundamental Physics, Astrophysics, Electronics, and Computing Sciences, at all university levels from undergraduate to graduate as well as at engineering schools. This maintains tight contacts with physicists, and sustains a steady flow of students with a strong background for internships and Ph.Ds at our lab.

### 1.1.5. Innovation and opening of new fields

A common quality of LERMA² scientists, encouraged by the laboratory diversity, is their originality of thought that leads to innovative developments and breakthroughs. Recent examples include (to name just a few):

- The first cosmological simulations with accurate radiative transfer, revealing how HI 21cm signatures of Reionization depend on the relative contribution of stars vs. quasars.
- The first convincing explanation, in terms of turbulent-driven non-equilibrium chemistry, of the long-lasting enigma of the ubiquity of $CH^+$ in diffuse interstellar gas.
- The discovery of *coreshine* in dense prestellar cores, a new powerful tool to probe the initial phase of grain growth and the initial conditions of protostellar collapse.

- The first demonstration of $NH_2OH$ synthesis (a precursor of amino acids) in cold interstellar conditions, using innovative laboratory experiments on ice substrates.
- The development of innovative instrumentation for high-resolution and high-accuracy infrared spectroscopy in the laboratory
- The combination of satellite survey data at different wavelengths to retrieve the global evolution of land surface flooding and humidity over the last 15 years.
- The innovative mixer design for the Channel 1 receiver of HIFI on board *Herschel*, which allowed an excellent sensitivity and stability together with a broad tuning range.

(Other examples may be found in the *Executive Summary* of the separate LERMA and LPMAA scientific reports).

### 1.1.6. Efficient dissemination of results through public databases

LERMA$^2$ members have developed a pioneering expertise in disseminating calculation results through public access databases, using advanced Virtual Observatory (VO) portals and visualization tools. The databases include tables of atomic and molecular data essential for astrophysical applications (collision rates, opacities, spectroscopic parameters, Starck broadening), and large grids of world-class numerical models for fitting observations (Galaxy mergers, MHD collapsing protostars, Photo-Dissociation Regions). LERMA$^2$ members are leading the development of new international VO standards to interoperate these databases, which will further enhance their impact in the community.

### 1.1.7. Applied developments and connections with the economic world

As a spin-up of Pole 4 R&D activities, LERMA$^2$ hosts one start-up company, *Estellus*, and develops joint projects with a few others, small (like *Artenum*) or large (like *Thales* or *Astrium*). We consider the use of our results in applied developments, as well as the recruitment of some of our former students by industrial partners, as real assets for the long-term.

## 1.2. Weaknesses

### 1.2.1. Geographic dispersion and difficulties in internal communication

The current lack of space on the Paris campus of Observatoire de Paris to accommodate any extra LERMA$^2$ members, and the need to keep tight links with our secondary partner universities, leads to the current dispersion of LERMA$^2$ over 5 geographical sites (OP-Paris, OP-Meudon, ENS rue Lhomond, UPMC-Jussieu, UCP-Cergy-Pontoise). The history of LERMA shows that this dispersion does not prevent major scientific achievements, helped perhaps by the fact that our 3 parisian sites are located within 20 minutes from each other. However, it does hinder informal day-to-day interactions, slows down synergies and collaboration projects, complicates management, and may even create misunderstandings due to the extensive use of email instead of direct contact.

*Proposed remedies:* LERMA$^2$ will dedicate special efforts to enhance internal communication across geographical sites. The new trans-site "Pole" management structure will strongly help, and a positive effect was already notable during the writing of the present quinquennial documents. This will be pursued by regular thematic Pole seminars or journal clubs rotating among sites, and by internal "blog" pages on the LERMA² internet site featuring news from each site and Pole. An official request for extra office space on the Paris campus of OP has also been made to accommodate LERMA² members from other sites and strengthen interactions, but the decision is not in our hands (see *Threats*).

### 1.2.2. Difficulties in external image and communication

Some of LERMA² strengths, namely its broad range of scales and techniques and its interface with Physics, also have a drawback: the lack of a simple identity as seen from outside. LERMA² emphasises the fundamental micro and macro-physical processes involved in the origin of cosmic structures of all kinds, more than one specific fashionable topic (*e.g.* hunt for exoplanets) or technical tool (*eg.* numerical simulations). We believe that this fundamental approach is a key to our major conceptual advances. However, this choice makes external public communication more difficult: towards the media of course, who are more responsive to a pretty image and simple idea than to an intricate spectrum; towards prospective students, who are influenced by fashionable topics and may have chosen astrophysics as an easier alternative to physics; and even towards our supporting entities and hiring committees, who are not always prepared to evaluate work at the interface between Astrophysics and Physics. Another challenge for our external image are the multiple geographical sites, which result in a diversity of formats and styles in the current LERMA website. We need to make a major progress in external communication to overcome these difficulties.

*Proposed remedies:* LERMA² will dedicate strong efforts to external communication through the nomination of a "communication team" in charge of advertising our activity and multi-disciplinary approach to the public and our supporting entities. The new LERMA² website, to be constructed during 2013, will be one key vector. The grouping of our research themes into 4 major thematic poles will also significantly help to sharpen our image.

## *1.3. Opportunities*

### 1.3.1. Integration of LPMAA and LERMA and transfer of LUTh-ISM members

The merging of the LPMAA and LERMA laboratories creates a strong research pole in molecular (astro)physics (Pole 3), where the sharing of expertise in theory and cutting-edge laboratory experiments is creating new synergies and research opportunities. This merging also reinforces the Pole 4 instrumentation capability for the development of space-borne instruments, with the strong expertise on balloon missions from LPMAA coming at the right time to support the new balloon experiment (CIDRE) proposed to CNES by LERMA. Finally, the arrival of two LUTh-ISM researchers is bringing new capabilities for modelling UV-irradiated molecular gas, and for building interactive VO modelling platforms. Combined with the LERMA² expertise in gas dynamics and gas-grain-photon interaction, this is the opportunity to create innovative and extremely powerful tools to interpret radio and infrared data on molecular regions in the MW and external galaxies (Poles 1 and 2).

### 1.3.2. New and planned major scientific facilities

The coming years are opening a "golden age" for radio-astronomy that represents a great opportunity for LERMA$^2$; Following the successful *Herschel* and *Planck* missions, which are still releasing new data products, ALMA has started its first operations. Thanks to our strong involvement in its conception (software and configuration optimization), we are optimally positioned to exploit this revolutionary instrument to study molecular regions with unprecedented detail and fidelity. The use of PdBI and its planned upgrade (NOEMA) is a further strong asset to optimize ALMA use. The e-VLA and LOFAR are promising similar breakthroughs in the cm radio range to study HI gas and ionized regions, while the approval of a microwave channel on the ICI satellite (Eumetsat) will also open a new era for ice cloud imaging studies. Finally, several planned instrumental projects involving other OP laboratories are opening new collaboration opportunities for LERMA$^2$ on 3D-mapping of the Galaxy (GAIA, with GEPI), Jupiterian system atmospheric physics (JUICE, with LESIA), re-ionisation of the Universe (SKA, with USN), and interaction of cosmic rays with magnetized interstellar clouds and supernova shocks (CTA, with LUTh). Conversely, the LERMA$^2$ expertise in *Herschel* and ALMA use will be shared with other laboratories of the OP through a transverse "Cercle de Competence" approved by the OP Scientific Council.

### 1.3.3. Participation in instrument projects

LERMA$^2$ is PI of the CIDRE balloon project, currently under a Phase A study financed by CNES, which is proposing to use new HEB design developed in Pole 4 to perform heterodyne spectroscopy of HD and OH at 2.7 THz. Pole 4 is also proposing to deliver the LO-chain for the Sub-millimetre Wave Instrument (SWI) on board JUICE, the next ESA mission to Jupiter's moons. Finally, the NOEMA project is opening new future opportunities for focal plane arrays, that we will contribute to through R&D activity on integrated SIS receivers. Such projects are important opportunities to maintain our technical expertise and collaborations (eg. with JPL or IRAM) at the highest level, to reward our R&D teams by concrete realizations, and to deliver cutting-edge data to our researchers.

### 1.3.4. Participation in "*Investissements d'avenir*" (2 IdEx, 6 LabEx, 2 EquipEx)

The LERMA, LPMAA, and their host institutions were very successful in the calls for the *Investissements d'avenir* launched by the previous French government. As a result, LERMA$^2$ is in the perimeter of two *Initiatives d'excellence campuses* (Idex): PSL (including OP and ENS) and SUPER (including UPMC), while its various Poles are partners in six *Laboratoires d'excellence* (Labex) and two *Équipements d'excellence* (Equipex). This examplifies the high level of in-house expertise of LERMA$^2$ over a wide range of domains, and its leadership capability (it initiated the Equipex MesoPSL and is coordinating the Labex Plas@Par). Such initiatives open new opportunities to attract outstanding students and academics, co-finance expensive equipments (eg. clean room, lasers, laboratory experiments), and strengthen our links with physics experts and other communities (eg. in supraconductive devices, Earth remote sensing, etc…).

### 1.3.5. New laboratory space on the Jussieu UPMC site

The expected delivery in 2015 of newly refurbished office and lab space in Jussieu for the Astrophysical Plasma team of Pole 2 will enable the development of new experiments in laboratory plasma astrophysics, and develop fruitful links with other plasma research and numerical physics activities on the UPMC campus. It is a much awaited opportunity.

## 1.4. Threats

### 1.4.1. Shortage of permanent research manpower

The founders of molecular astronomy in LERMA$^2$ (P. Encrenaz, M. Guélin, J. Lequeux, E. Roueff, N. Feautrier, E. Falgarone …) have reached retirement age, or will do so during the next reporting period. Although we have been quite successful at attracting new talents, two of our most prominent scientists have accepted in 2012 more attractive job offers, with less teaching duties and higher salaries (S. Balbus in Oxford, P. Hennebelle at CEA). In addition, most of our recent recruitments are on teaching positions (CNAP or university) whereas most of our retiring members are full-time researchers from CNRS. Although this imbalance is partly compensated by an increase in short-term contracts funded by national and European grants (ANR, ERC, Marie Curie…), the latter are restricted to starting young researchers (students or young post-docs) and thus need to focus on relatively "safe" and short-term results. This situation is creating a threat on our excellence level and innovation capacity, since the fundamental LERMA$^2$ approach of combining micro and macro-processes requires a long training, and ambitious or risky projects require many years of dedicated development efforts. This is particularly true for example in heavy radiative-MHD simulations, physico-chemical modelling, and laboratory experiments.

*Remedies:* LERMA$^2$ does not have a direct hand on research staff hiring, which is decided by our supporting entities (CNRS, CNAP, and university); however we list in section "Project Implementation" the researcher profiles that our thematic Poles consider as top priorities for recruitment over the next period, to maintain our excellence and innovation capability. In particular we also hope that ENS will reopen the astrophysics chair at ENS as soon as it is definitely freed by S. Balbus, to attract a prominent scientist with high level in both physics and astrophysics capable of leading innovative ambitious projects and enhancing synergies among Poles, in close interaction with the Physics Department.

### 1.4.2. Shortage of permanent engineer manpower

Several technical areas where we have gained international leadership and deliver essential services to the community are under threat, as they currently rely on non-permanent engineering positions:

- The infrastructure for VAMDC (Virtual Alliance for Molecular Data Center) is developed by a software engineer financed by an FP7 European grant that will end in 2014.
- The FORMOLISM experimental platform for surface reactivity in Cergy–Pontoise is managed by an engineer under short-term contract with UCP (S. Baouche).
- critical new analysis tools and databases required for Earth remote-sensing in the (sub)mm range are developed by a highly talented engineer under short-term contract.
- The interactive "ISM and Jets" OV platform developed by F. Le Petit for modelling molecular regions, considered as an essential service by the PCMI and PNPS communities, relies on the key technical expertise of an engineer assigned to a

different laboratory (LUTh).

- The adaptation of codes to increasingly powerful machines and the display of the huge sets of simulation data require more and more advanced technical expertise in HPC, that requires support from a highly trained professional engineer.

*Remedies:* We give in section “Project Implementation” of this report a tight recruitment plan with the engineer profiles that our thematic Poles consider as top recruitment priorities over the next period to secure our experimental and service capacity.

### 1.4.3. Shortage of office space

Our current premises on the Paris site of OP have overflown maximum occupancy threshold, and cannot accommodate the growing number of students, post-docs, and visitors of Poles 1 and 4, nor any LERMA² members from other sites. This situation is threatening the day-to-day functioning of the lab, as well as its internal synergies and its development. Additional office space on the Paris site is urgently needed and a corresponding request has been sent to the OP President.

The ENS buildings located 24 rue Lhomond will undergo complete renovation work, starting mid-2013 for a period of at least 2 years. The LERMA² offices at ENS are particularly threatened by this renovation, as part of them will be turned into public areas and open spaces. To maintain the high attractiveness and visibility of our ENS group on MHD simulations and chemical modelling of inter/circumstellar gas, and the very fruitful and stimulating interactions it has developed within the ENS Physics Department, re-attribution of equivalent office space in the refurbished ENS building will be necessary.

### 1.4.4. Support of our fundamental physics activities

As noted above, one strength and originality of LERMA² is its interdisciplinary approach combining Astrophysics and Physics. An important drawback is that fundamental molecular and plasma physics are not within the priorities of our governing CNRS Institute INSU (Universe Sciences) nor in those of Observatoire de Paris. Funding and manpower support in this area thus relies heavily on our other university partners. LPMAA currently benefits from a strong support from its governing CNRS institute INP (Physics), which has been playing an essential role in its development. The switch of LPMAA from INP to INSU perimeter, following it merging with LERMA, is then a serious threat for this team. The success of the newly merged laboratory will require that INP (and of course UPMC) guarantees to keep the same level of support to these fundamental molecular physics activities, as done eg. by INP for SYRTE for their fundamental metrology activities. Likewise, our strongly interdisciplinary activities, such as laboratory plasma astrophysics, will not develop unless they obtain simultaneous support from both contributing CNRS institutes.

# 2. Pole 1: Galaxies and Cosmology

***Permanent staff**: F. Combes, F. Debbasch (1/2), J.-M. Lamarre, A.-L. Melchior, P. Salomé, N. Sanchez, B. Sémelin, D. Valls-Gabaud, F. Viallefond (1/2), M. Wiedner (1/2) ; affiliated researcher: H. de Vega.*

***Non permanent:** M. Bahi, P. Beirao, M. Bois, K. Dasyra, J. Freundlich, A. Halle, S. Hamer, V. Lattanzi, G. Novak, J. Scharwächter, M. Stringer, J. Vega, C. Verdugo*

## 2.1. Scientific originality and strategic evolution

The thematic Pole, specialized in the study of galaxies and Cosmology, includes 10 permanent researchers, and a dozen of post-docs and students. They work both in the field of observations and theory, and are experts in numerical simulations. The strengths of the group are:

(1) the study of the physical and baryonic processes: radiative transfer, formation of stars and feedback, fueling of black holes, in addition to the dynamics of dark matter.

(2) the very tight confrontation between theory, simulations and observations;

(3) the strong involvement in present and future international projects; Herschel, Planck, ALMA, SKA...

The group will continue tu work on original topics, such as radiative transfer in the Early Universe, for which only a few groups have expertise in the world, high redshift galaxies or cooling flows, with the goal of further breakthroughs at the forefront of the research, and very deep physical insight in nearby galaxies, tackling phenomena like mergers, radial migration, AGN fueling and feedback, the role of secular evolution and cosmic accretion in galaxy mass assembly.

## 2.2. Cosmology and Early Universe

### 2.2.1. Cosmic microwave background (CMB)

*Lamarre,*

The **Planck HFI** Instrument Scientist, and several LERMA researchers, are involved in the Planck working groups. The main purpose of the mission is to map the CMB anisotropies and to test the theory of inflation. But Planck also provides an allsky survey at mm and submm wavelengths, and a catalogue of sources at various redshifts. The work on Planck foreground emissions has developed strong synergies with Pole 2.

In January 2012 the high frequency (HFI) instrument completed its observations, and many early results were published in a special issue. Publications on the CMB should begin in 2013, and will continue into 2014, first without polarization, then with all calibrated data, with catalogues of compact sources, and the measurements of the Sunyaev-Zeldovich (SZ) effect in clusters in 2015.

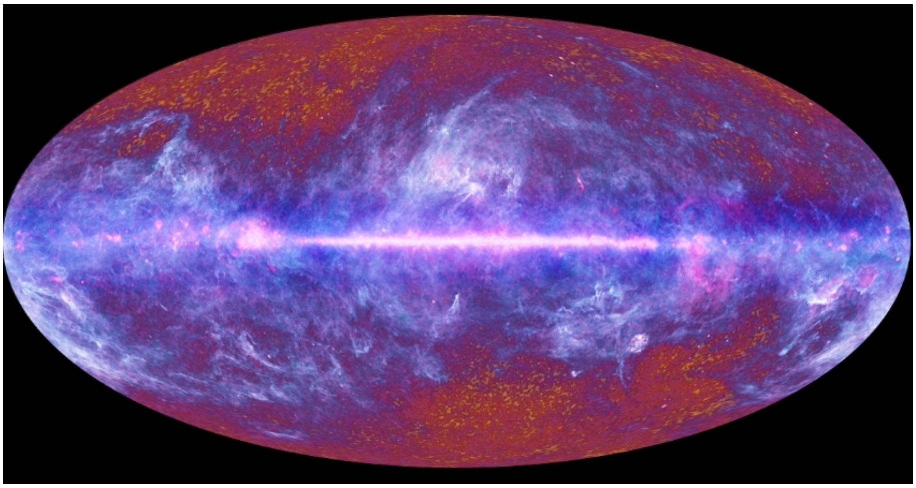

*Fig. 2.1: This image from Planck shows the dust and gas emission of our Galaxy in blue, pink and white – most conspicuously the galactic disc across the middle of the image. At the top and bottom, the red and yellow mottled areas display fluctuations of the Cosmic Microwave Background (CMB).*

### 2.2.2. Inflation models

*Sanchez, de Vega*

One group working on the Standard Model of the Universe proposes a universal shape for inflationary potentials and their couplings. Such models allow to predict the ratio between fluctuation amplitudes of tensor and scalar fields. This ratio, dependent on the importance of primordial gravitational waves is a test for models of inflation. One of the problems detected in the CMB is the low observed level of the quadrupole component. The models in LERMA have been generalized to account for the low observed CMB quadrupole. In the next years Planck results on the CMB combined with the study of large scale structures will test the assumption of a 2-minima potential for the inflaton, and allow to derive the scale of inflation.

### 2.2.3. Dark matter

*Combes, Sanchez, de Vega*

Two LERMA teams study the **problem of dark matter**, which has been around for dozens of years, but appeared in more acute terms recently: the standard Λ-CDM model of cold dark matter cannot account for observations on galactic scales, as it predicts too much dark matter concentration in galaxies (core-cusp issue), and too many satellites for large galaxies. The alternatives are studied theoretically and with the help of simulations: hot or warm dark matter (classical or sterile neutrinos), modification of gravity. The comparison with observations and the development of simulations and theoretical work will provide constraints on the various possible models.

### 2.2.4. Epoch of Re-ionization (EoR)

*Sémelin, Combes, Viallefond*

Another team of Pole 1 is carrying out simulations of the **Epoch of Re-ionization (EoR),** time corresponding to the first stars and early galaxies, whose UV radiation are going to re - ionize the Universe between z = 30 and z = 6. Observation of the HI line of atomic hydrogen at 21-cm redshifted into metric waves will be performed soon with LOFAR, and in a more remote future with SKA. The LERMA simulations predict what types of structures will be easier to detect, and are very useful to optimize the design of SKA. The scientific challenge is to better understand the first structures in the Universe, galaxies and quasars. The simulations deal with the dynamics of the formation of galaxies, but also with a sophisticated radiative transfer that takes into account the UV photons, the X-rays, and all the Lyman lines, which allow to couple the excitation temperature of atomic hydrogen to its kinetic temperature. A wide range of scales is necessary in these simulations, and they will progress from $512^3$ to $1024^3$ and $2048^3$. The team also develops HI tomography analysis to enable a better interpretation of the data when they arrive.

### 2.2.5. Fundamental constants

*Combes, Lattanzi, Salomé*

Grand unification theories, non-standard models of dark energy, quintessence, Chamaeleon theory etc .. each predict **a variation of fundamental constants**, either temporal or spatial variations. Observations in radio-astronomy, with unmatched spectral resolution, allow to constrain these variations, thanks to molecular absorption lines in front of distant quasars. The LERMA group is very competitive in this area, and will continue to observe with IRAM and ALMA in the future, with progress expected thanks to the increased sensitivity, and the extra-wide frequency bands, which allow spectral surveys.

## *2.3. Formation and Evolution of Galaxies*

### 2.3.1. Star Formation in High Redshift Galaxies

*Combes, Dasyra, Freudlich, Salomé*

A LERMA team works actively on the observation of **galaxies at high redshift**, to follow in real time their formation and evolution, and compare the observations to theory and simulations: the challenge is to know the efficiency of star formation, understand the history of this formation over cosmic time, understand why the most massive galaxies are active at the beginning of the universe, while today the most active are mainly dwarf galaxies. The team is leading some key projects at IRAM, Herschel, and prepare programs on ALMA, which will become fully operational in 2013. All wavelengths are used to characterize the objects that are selected either by their infrared emission (Herschel), then detected in their molecular gas, imaged in optics with the Hubble Space Telescope, with a spectroscopy done on large telescopes on the ground (VLT, Keck..). Gravitational lenses are systematically used to increase the spatial resolution of very distant objects.

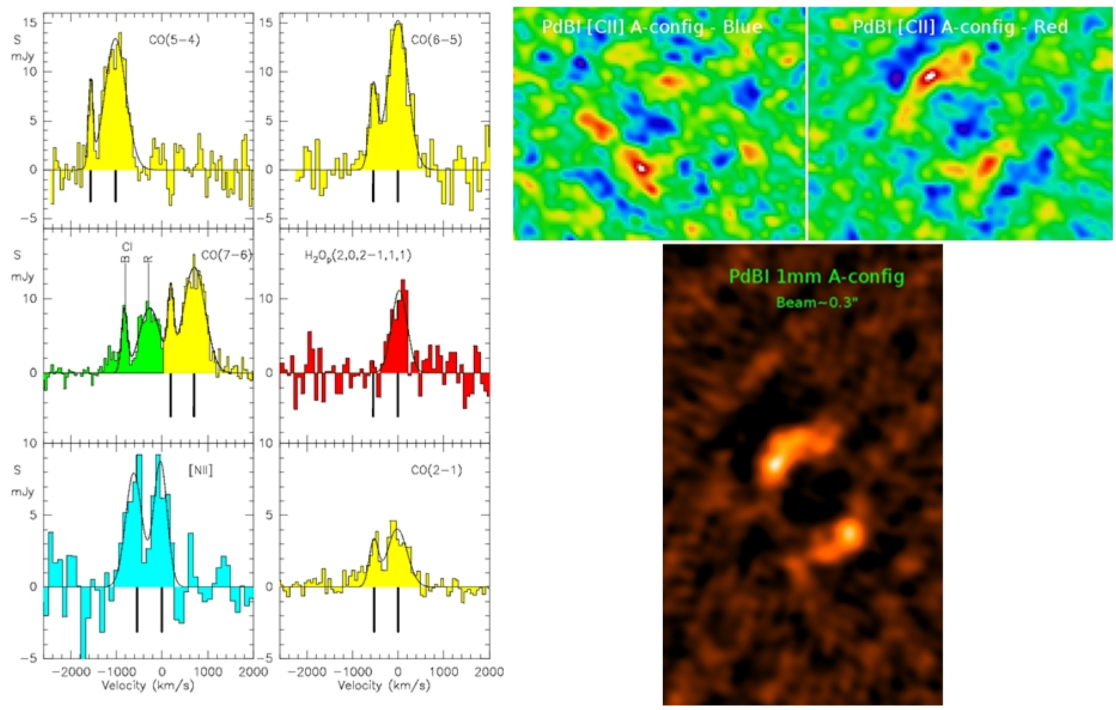


*Fig. 2.2: Example of a galaxy at z=5.243 discovered with Herschel, with its redshift determined with CO lines at IRAM-30m. The left image shows the various CO spectra, with also water, CI and [NII] lines. The right images reveals arcs from the gravitational lensing, both in the C+ lines and in the continuum with PdB.*

### 2.3.2. Galaxy mergers

*Combes, Melchior, Sémelin, Bois, Stringer, Dasyra*

The LERMA group has contributed to the achievement of the **galaxy mergers library GALMER**, which allows the study of physical phenomena related to the hierarchical galaxy formation: dynamically triggered starbursts, counter-rotating systems, exchange of angular momentum. In the future, these simulations will be carried out with a spatial resolution and particle mass resolution well above the present, and new phenomena associated with the star formation and feedback, and the presence of active galaxy nuclei (AGN) will be described more realistically, to clarify their role in the evolution of galaxies.

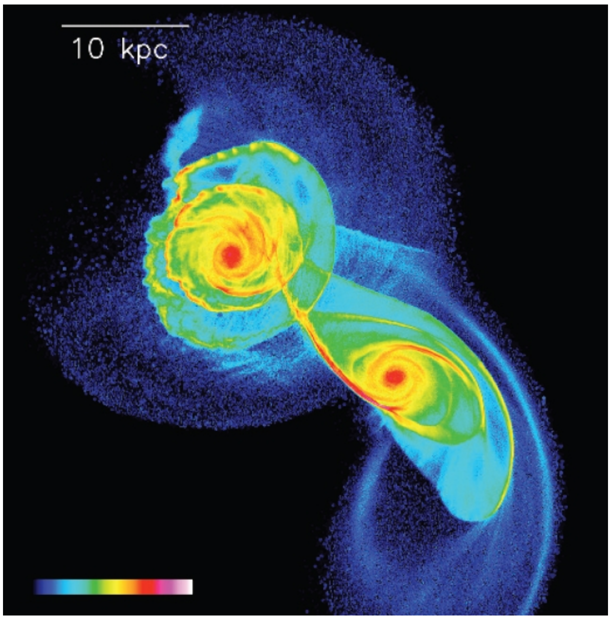


*Fig. 2.3: High resolution (30 millions of particles) of a galaxy merger, from the GALMER database.*

### 2.3.3. Active Galaxy Nuclei

*Dasyra, Combes, Novak, Beirao, Scharwächter*

Models will be constrained by the comparison with observations of the behaviour of gas in nearby galaxies **with active nucleus (AGN)**. Observational campaigns are already underway with ALMA cycle 0, and will grow considerably in the coming years. In particular, the presence of the streams of gas ejected at high speed by active nuclei will be sought and studied, in order to compare with the associated feedback patterns described in the simulations. The challenges are to better understand the association between supermassive black holes and galaxies bulges, and its cosmic evolution.

### 2.3.4. Cooling flows in clusters

*Salomé, Combes, Hamer*

LERMA Pole 1 is also widely recognized for its work on **cooling flows**, both by its first observations of cold molecular gas, and its simulations of physical processes. The team participates in key programs on Herschel to observe cooling elements such as C+ and OI, and ongoing projects on ALMA cycle0. In the future ALMA in full operation will be able to make large progress on the nature of the multi-phase filaments of ionized gas and cold molecular gas. Modelling further with photo-ionization codes as CLOUDY and numerical simulations of the possible dynamical scenarios will be performed (shocks, heating by stellar formation, or by cosmic rays).

### 2.3.5. Physics of Nearby Galaxies

*Melchior, Valls-Gabaud, Viallefond, Combes, Bois, Beirao, Hallé, Verdugo, Wiedner*

Another of the specialities of the group is the **physics of nearby galaxies**, treated both by modelling, numerical simulations and observations: what is the respective role of secular evolution, of galaxy interactions, in star formation and its efficiency? The comparison with observations involves infrared emission from dust, or recombination lines, as tracers of stellar formation, and molecular gas. The interpretation of the Kennicutt-Schmidt law, local or global, is one of the challenges of these studies, which will improve considerably with the spatial resolution and sensitivity of ALMA. All types of galaxies will be studied, dwarfs, ellipticals as well as spirals, and the CO -to- H2 conversion factor will be known with more details and statistics. The effects of environment, ram pressure, tidal forces, harassment or removal of the gas supply, will be studied.

The numerical simulations will be also developed to study various scenarios of formation of galaxies like the Milky Way, the roles of secular evolution with accretion of gas from the cosmic filaments, or interactions/mergers (minor or major) to reproduce abundance gradients, the formation of galaxy disks without bulge or pseudo-bulge, the formation of thick disks, the migration of stars. The evolution of these processes in cosmic history will be developed.

## 2.4. Conclusion

In summary, Pole 1 will develop projects in the following main directions, with observational, modelling and theoretical approaches:

- The Early Universe: inflation, cosmic backgrounds, re-ionization.
- Dark matter: cold, warm dark matter or modified gravity.
- Galaxy formation: high-z, early galaxies, secular evolution and mergers.
- Black holes and galaxies: AGN, starbursts, symbiotic growth and feedback.
- Star formation efficiency, history and stellar populations.

Clearly synergies will further develop with Pole 2 on improved approaches to dissipative processes impacting the dynamics of galaxies, with Pole 4 on the development of new concepts for structuring and accessing the large databases constructed from numerical simulations, and in a much transverse way within LERMA on methodological developments to enhance the use of new generation instruments and computers.

# 3. Pole 2: Dynamics of the ISM and Stellar Plasmas

*Besides intervening recruitments, Pole 2 in 2014 will be composed of 24 permanent researchers distributed among: 9 full-time CNRS researchers (M. Gerin, T. Le Bertre, P. Lesaffre, J.-F. Lestrade, L. Pagani, M. Pérault, L. Petitdemange, C. Stehlé, C. Zeippen), 5 university teaching staff (A. Ciardi, F. Debbasch (50%), F. Levrier, J.-F. Panis, L. Tchang-Brillet (50%)), 5 « astronomes » CNAP (S. Cabrit, F. Delahaye, M. Heydari, F. Le Petit, J. Pety), and 5 emeriti (E. Falgarone, M. Guélin, J.-L. Lequeux, E. Roueff, S. Sahal-Bréchot). It will also have 4 external research associates from nearby institutes (G. Pineau des Forêts from IAS, E. Dormy from IPGP, P. Hennebelle from CEA/IRFU, J. Le Bourlot from LUTh), and one frequent visitor (A. Meftah). Based on the current situation in 2012, we also expect around 10 Ph.D. students and 5 postdocs at any time. In addition 2 technicians and engineers are expected to participate: N. Champion (50%), C. Blaes (50%).*

## *3.1. Scientific originality and strategic evolution*

Pole 2 works towards solving outstanding fundamental issues in ISM and stellar physics: (1) understanding the key steps in the ISM condensation path leading from turbulent atomic diffuse gas to dense prestellar cores, stars, disks and planetary systems, (2) understanding the feedback of accretion-ejection processes onto the ISM cycle and star formation, (3) understanding the structure and evolution of dusty accretion discs and stellar interiors subject to complex turbulent and radiative transport processes. As described in the "Results" document, Pole 2 has developed several specific strengths that make it particularly competitive in these areas:

- Observations: A long-established expertise in sub/millimetric observations and interferometry, whereby Pole 2 has earned a leading international role in *Herschel, Planck (Galactic Foregrounds)*, IRAM, and an already substantial involvement in ALMA Early-Science; and the access to multi-wavelength studies from the FUV to the cm range, thanks to strong international collaborations (VLT, HST, e-VLA, SOFIA…).
- Modeling: A world-class expertise in MHD turbulence and high-resolution 3D MHD codes and simulations, with a pioneering role in new improvements for more realistic results (eg. radiation diffusion, non-ideal effects…); Original models of non-equilibrium chemistry and heating/cooling coupled with gas dynamics (vortices, shocks, jets), with no equivalents worldwide; and the full mastering of radiative transfer tools and instrument simulators to make synthetic predictions comparable to observations (eg. for ALMA).
- Fundamental physics and laboratory experiments: The local development and mastering of accurate theoretical tools, and the access to numerous national and international state-of-the-art facilities (Z-pinches, kJ lasers, SOLEIL synchrotron, VUV spectrometer in Meudon) which allow us to identify and explore new processes, and complement / benchmark numerical simulations and theories.

Another original strength of Pole 2 is its ability to *combine* several of the above approaches to, eg., design new observational/experimental tests of proposed theories or, conversely, to rapidly translate recent observational/experimental discoveries into original and well adapted modelling avenues. This multi-methodology approach is also enriched by close interactions with physicists working on e.g. plasmas, turbulence, and dynamos, through the LabEx structures Plas@par at UPMC (coordinated by a Pole 2 member) and ICFP at ENS.

These unique strengths put us in an optimal position to take full advantage of the new observatories and experimental facilities coming on-line, and extract key understanding on the ISM cycle and star/disk/planet formation. For this, it is also necessary that we maintain sufficient manpower. Our chemical modelling tools will broaden in 2014 by the transfer to LERMA[2] of two members of the LUTh-ISM group (F. Le Petit and E. Roueff) bringing top-level expertise in UV-irradiation that complements our own (turbulence, shocks) and enables a more realistic modelling of ISM chemistry. On the other hand, our most experienced researchers in ISM modelling and observations, who have been playing a key role in this domain, will have reached emeritus/retired status (Falgarone, Pineau des Forêts, Roueff). Given the huge inflow of new data brought by *Herschel, Planck*, and then ALMA, NOEMA, and JWST, we will clearly need to recruit two young researchers in 2014-2018 to maintain the Pole 2 manpower and international leadership in physico-chemical modelling and ISM observations. Two members of the MHD group at ENS were also offered positions in June 2012 at other institutes, with higher salary and less teaching duties (the Savilian chair in Oxford to S. Balbus, and a full research position at CEA/IRFU to P. Hennebelle). Although they wish to maintain links with Pole 2 through joint projects (e.g. ANR COSMIS) and co-supervision of Ph.D. students, their replacement will be crucial to maintain our international leadership in MHD.

## 3.2. Observational characterization of the ISM cycle

The tremendous success of the *Herschel* and *Planck* space missions, combined with the continuous improvements of the Plateau de Bure Interferometer (PdBI and its planned extension NOEMA), and the completion of ALMA in 2013, are opening a « golden age » for european (sub)millimetre astronomy. The challenge for the future is to take the best advantage of these facilities to tackle the « hot » scientific questions emerging from early results. Our team is already collaborating to about 30 new accepted projects on these instruments (about 20 on *Herschel*, 5 on PdBI, 5 on ALMA Early-Science), so that we are optimally positioned to address the following key issues over 2014-2018:

### 3.2.1. How does turbulence dissipate, and where?

*Falgarone, Pety, Godard*

Interstellar turbulence can dissipate in shocks, intense velocity shears, and current sheets, all of them being small-scale structures barely accessible to current instruments. Turbulent dissipation may now be searched for at very small scale with unprecedented sensitivity with ALMA and NOEMA. The impact of turbulent dissipation is not limited to the diffuse ISM but will also be investigated in the context of dense cores, circumstellar disks, photo-dissociation regions, and at larger scales in external galaxies. We will focus on the properties of CO, which is the main tracer of molecular mass in the Universe, but will also explore the newly established chemical diagnostics of warm chemistry in the diffuse medium (see below).

### 3.2.2. What are the topology and intensity of interstellar magnetic fields, and what is their impact on star formation?

*Falgarone, Levrier, Hennebelle*

The *Planck* satellite is producing the first full sky map of polarized dust emission: it is unexpectedly high. We are involved in six (and lead one) studies of *Planck* galactic polarized foregrounds. Our MHD numerical simulations (see below) will provide a unique and quantitative tool to analyse these data, i.e. to characterize the large-scale ordered magnetic field and disordered turbulent component, and to reveal the role of the large-scale field in determining cloud structure and star formation activity. To probe the field on the smaller scale of filaments, cores and circumstellar regions, we are also leading a pioneering international program on dust and Zeeman polarization studies with IRAM-30m and SMA, which will continue on ALMA and NOEMA once these new facilities are properly equipped. These will be used to distinguish among various models of magnetized protostellar collapse and disk/outflow formation.

### 3.2.3. When is dust growth to micron-sizes occuring in dense cores?

*Pagani + Ph.D. student*

Grain growth must be better characterized observationally, since it modifies the temperature, ambipolar diffusion, and chemistry in the (pre)collapse phase, and increases the potential for planet formation. The *Spitzer* archive revealed the "coreshine effect" in only 50% of prestellar cores, and 75% of older cores containing protostars. To clarify the conditions favoring grain growth, a new study of 100 cores sampling a broader range of properties was accepted on warm *Spitzer*, completed by ground-based and *Herschel* data, and detailed radiative transfer modeling (new Ph.D. thesis directed by L. Pagani). This will pave the way for JWST, which will be able to map "coreshine" at 0.2" resolution and infer the detailed internal structure of prestellar cores.

### 3.2.4. What are the various chemical pathways operating in the ISM ?

*Gerin, Pagani, Roueff*

*Herschel* and IRAM are revealing strong variations in isotopic fractionation and ortho-para ratio (OPR) among different molecules and different environments, pointing to a diversity of chemical formation paths. Systematic line surveys are the best way to test proposed chemical models (in synergy with Pole 3) in a complete and unbiased way; Thanks to huge progress in receiver bandpass and stability, these surveys can now be performed relatively easily from the ground, and our team will be playing a leading role in exploiting the ongoing IRAM line surveys of the Horsehead nebula PDR (PI: Pety, ANR SCHISM) and of a variety of nearby cores / protostars (PI: Lefloch, IPAG).

### 3.2.5. What is the physical link between accretion and ejection, and the feedback on star and planet formation ?

*Cabrit, Roueff, Lestrade*

We will clarify the frequency, dynamics, chemistry, and role of protostellar jets in early star / disc formation through an accepted large survey of protostellar jets/sources at PdBI (CALYPSO, PI: Ph. André) and complementary ALMA and SOFIA projects, in collaboration with Chile and Germany. The deployment of a new generation of UV-optical-IR spectrometers on the VLT (SINFONI, MUSE, XSHOOTER) and HST (COS), then E-ELT, also opens new fantastic opportunities for studying ejection and accretion signatures in less embedded T Tauri stars. In particular, we will pursue our collaboration with K. France et al. (USA) on FUV fluorescence from $H_2$ and CO in discs, which probes the irradiated disk surface and may be crucial to the interpretation of *Herschel* $H_2O$ and [OI] data on these sources. Studies of debris discs will strongly benefit from the increase of sensitivity on IRAM (NIKA) and the start of NOEMA and ALMA, to improve the detection statistics and probe the dust structure at high spatial resolution.

### 3.2.6. How do massive stars form ?

*Heydari-Malayeri, Salomé*

The process of massive star formation and its dependence on metallicity and environmental conditions (OB cluster vs isolated) are still unsolved open problems. To gain new clues on these issues, we will pursue our study of massive protostar candidates in the Magellanic Clouds (MCs). We will combine HST observations with new ALMA data in $^{12}CO$(3-2), CS(7-6), $HCO^+$(4-3), HCN(4-3), $^{13}CO$(1-0), and $C^{18}O$(1-0) to assess their evolutionary stage, their outflow properties, and the physical conditions in their parental clouds in unprecedented detail. We will also observe with VLT and ALMA some recently identified candidates for isolated massive star formation, such as SMC-N33 (Selier et al. 2011).

### 3.2.7. How is enriched stellar matter ejected and mixed into the ISM ?

*Le Bertre*

Evolved stars expel their newly synthetized elements through dense winds that are a major contributor to ISM enrichment in heavy elements and dust grains. The expanding shells are then slown down by ambient pressure and eventually disrupted, for instance in turbulent wakes where stellar matter mixes with the ISM. We will use CI and [CII] data recently obtained with *Herschel*/HIFI, and HI 21 cm data obtained with the e-VLA and SKA precursors such as MeerKAT, in order to constrain the kinematics in the turbulent wakes, which remain poorly studied observationally. We will also investigate the inner molecular wind structure with IRAM (NOEMA) and ALMA, eg. in CO. This will prepare the exploitation of higher angular resolution data to be obtained in 2018-2020 in the near-infrared by the Indian space project IRSIS, and in the sub-millimeter range by the SAFARI instrument on SPICA.

Finally, the strong participation of Observatoire de Paris in the **GAIA mission** offers the opportunity to share our expertise with the GAIA team to determine the 3D structure of the ISM. This joint action, led by R. Lallement (GEPI), is part of a proposed FP7 EU project (PI N. Walton, UK).

## *3.3. Modelling chemical diagnostics of ISM dynamics*

NB: to disseminate our knowledge of ISM structure and evolution towards a broad (extra/galactic) community, the models described below will progressively be made publicly available on the "ISM-platform" of the VO-portal at Observatoire de Paris.

### 3.3.1. Turbulent Dissipation Region (TDR) models

*Momferratos (Ph.D.), Falgarone, Lesaffre, Pineau des Forêts (associate)*

To accurately model the chemical impact of turbulent dissipation in the ISM, and to correctly interpret spatially unresolved observations (eg external galaxies), a new generation of more realistic models of chemical dissipation regions needs to be developed, beyond the already complex 1D approach elaborated by Godard et al (2009). This is the goal of the Ph. D. thesis of G. Momferratos started in Sept. 2010, co-supervised by E. Falgarone and P. Lesaffre. Incompressible 3D MHD simulations with viscosity, resistivity, and ambipolar diffusion are being conducted to analyse the different types of dissipative structures. The next step will be compressible 3D MHD simulations with RAMSES, including a robust chemical network of about 40 species previously tested in 2D and optimized for the time-scales imposed by the MHD. The results will yield predictions of molecular line profiles for comparison with observations of turbulent regions.

### 3.3.2. Photon Dominated Region (PDR) models

*Bron (Ph.D.), Le Petit, Roueff, Gerin, Le Bourlot (associate)*

The "Meudon" PDR code has become a reference for a large community (the 2006 release is cited 130 times). Updating its microscopic processes is mandatory for a realistic interpretation of more and more detailed observations, including that of external galaxies (synergy with Pole 1). The most timely project is the detailed inclusion of gas – surface interactions (reactions, photodesorption), based on recent theoretical and experimental achievements (synergy with Pole 3). Heating processes for the grains and gas are also being improved as part of E. Bron's Ph.D. thesis. In a collaboration with C. Joblin (IRAP), PDR models are further modified to take into account the size evolution of the smallest grains, which has a profound effect on both the penetration of UV radiation and the gas photoelectric heating. This leads to stronger high-J CO line emission than in standard PDR models, in closer agreement with *Herschel* observations. The PDR model will also be extended to include the effects of turbulence, and of high energy radiation (X-rays & cosmic rays) which is essential to model protostellar disks, SNRs, and gamma-ray-burst host galaxies (where a significant amount of molecular gas has been detected at large redshifts).

### 3.3.3. MHD shocks and jet models

*Gusdorf (post-doc), Lesaffre, Cabrit, Pineau des Forêts (associate)*

Our *Herschel* discovery of very broad $CH^+$ line wings in DR 21 (Falgarone et al. 2010) required the development of new MHD shock models including FUV irradiation, in which $C^+$ could react with warm $H_2$. A first model for average irradiation was validated on $H_2$ shock observations in the Stefan Quintet (Lesaffre et al. 2012). The reaction network will now be completed (with the help of PDR models) to handle higher UV fields, and applied to model the irradiated molecular shocks occurring in massive star forming regions observed with *Herschel* (PRISMAS program) and at the base of young protostellar jets observed with *Herschel* (WISH program), PdBI and ALMA. Such shocks have been invoked as the origin of high-J CO emission up to J=40 in some protostars, but self-consistent models are still lacking and absolutely necessary to test this hypothesis. MHD shock modelling in supernovae remnants (SNR) has also been started by A. Gusdorf as a means to constrain the locally enhanced cosmic-ray flux (link with the ANR COSMIS). Photodissociation by Lyα produced within the shock itself will also be investigated, as it might explain the low $H_2O$ / OH ratios suggested by *Herschel* observations of some shocks located far from any ambient FUV field.

### 3.3.4. Coupling MHD simulations, (polarized) radiation, and chemistry

*Valdivia (Ph.D.), Commerçon (post-doc), Falgarone, Levrier, Hennebelle (associate), Pérault*

An urgent challenge is the self-consistent coupling of time-dependent gas dynamics with radiation. Our group was the first to carry out 3D MHD fluid simulations of protostellar collapse including the feedback of radiation transport (Ph.D. thesis of B. Commerçon). We also developed a tool to produce realistic synthetic observations, by an interface coupling the output of simulations to radiative transfer codes and instrumental simulators. We are already able to compute synthetic ALMA dust continuum maps of collapsing cores (Commerçon, Levrier, et al. 2012; in press), and the extension to line emission is underway (collaboration with LAB/OASU). Modelling of the *Planck* foreground ISM polarization will involve similar developments in numerical simulations, including prescriptions for the dust alignment on the magnetic field by radiative torques as a function of UV-shielding and gas density, coupled with advanced processing tools able to make quantitative predictions of the emergent polarized signals. Another urgent question is the effect of time-dependent irradiation and dynamics on chemistry. This is addressed by a new Ph.D. student, V. Valdivia (2012-, co-supervised by E. Falgarone and P. Hennebelle) who will introduce a self-consistent treatment of UV irradiation and (simple) chemistry within large-scale 3D simulations of turbulent clouds. This approach will enable to test the validity, in turbulent and non-homogeneous media, of usual diagnostics of ISM physics such as the determination of the cosmic ray ionisation rate from $H_3^+$.

### 3.3.5. Chemical models of fractionation and ortho-para ratio in the ISM

*Gerin, Pagani, Roueff*

Because the cold temperature and presence of UV radiation favour isotopic fractionation processes, the isotopic enrichments in D/H or $^{15}N/^{14}N$ in molecules may be used as probes of chemical processes in specific environments. Our recent models have shown the importance of symmetry states in the reactivity, and the next challenge is the development of a complete chemical network including symmetries both in the gas and solid phases. As many processes are still poorly modelled, or lack quantitative measurements, the development of such networks by Pole 2 will strongly benefit from our close synergy with physicists (in particular in Pole 3). Particular attention will be paid to nitrogen chemistry ($^{15}N/^{14}N$ ratio), which remains less well understood than C and O chemistry. These models will be applied to the large spectral surveys of various regions now ongoing with IRAM-30m.

## *3.4. Laboratory plasma experiments*

### 3.4.1. Magnetized protostellar accretion and ejection

*de Sa (Ph.D.), Chaulagain (Ph.D.), Ibgui (post-doc), Ciardi, Stehle, Cabrit*

Our main objectives will be to clarify the launching and collimation mechanism of protostellar jets, and to probe the angular distribution of the UV and X-ray radiation emitted by the jet base (through reconnection) and by the accretion shock (PhD thesis of L. de Sa co-supervised by C. Stehlé and J.P. Chièze from CEA/IRFU). Both processes have strong consequences for models of disc evolution and planet formation.

Our approach combining experiments and numerical simulations of laboratory and astrophysical jets and shocks will be developed along 3 main axes: 1) with the CEA-Gramat Center, we shall extend the studies performed on the MAGPIE Z-pinch facility to larger plasma volumes, and longer time-scales, to study for example, the development of instabilities in the jet-ambient medium interaction that cannot be followed numerically to such accuracy; 2) with LULI (ANR SILAMPA starting in 2013), we will investigate the collimation of wide-angle flows into jets by *a static ambient field*. These are the first experiments ever to couple a strong, steady-state, magnetic field (up to 0.4 MG) with a laser-produced plasma, allowing to study both jets and accretion columns; 3) with LPP, we will study shocks in yet unexplored regimes (shocks cooled by radiation, magnetized shocks), using a newly implemented conical plasma focus at LPP (100kA) able to launch shocks at 20 kms/s over more than 1 cm. This work complements the study of shocks generated by high-energy laser facilities, which is the subject of the on-going Ph.D. thesis of U. Chaulagain.

The physical understanding developed in laboratory experiments will be scaled-up to model astrophysical cases and their expected spectral signatures, in synergy with observational experts in Pole 2. To support these studies, we will not only develop our expertise in 3D numerical simulations adapted to both laboratory and astrophysical plasmas (MHD and 3D radiative transfer), but also acquire additional expertise in radiation hydrodynamics and in hybrid particle-fluid models.

### 3.4.2. VUV Spectroscopy of heavy ions

*Tchang-Brillet, Meftah*

Experimental and theoretical investigations of VUV spectra from heavy element ions will continue together with critical compilation of existing data by isoelectronic sequences. We will benefit from a newly purchased high-resolution scanner on image plates, providing linear intensity measurements extending down to 195Å. These studies provide fundamental parameters for stellar atmospheres and magnetic fusion plasmas, and for cosmochronometry. The determination of experimental energy levels will contribute to improved calculations of opacities, for the iron group elements for instance.

## 3.5. Transport mechanisms in stellar plasmas

### 3.5.1. Rotating stellar interiors and discs: convective instability and dynamos

*Raynaud (Ph.D.), Lesaffre, Petitdemange, Dormy (associate)*

Helioseismology recently revealed a complex rotation profile in the Sun's convective zone, with no spherical or cylindrical symmetry. Hence, there is a pressing need for stellar evolution codes to include a self-consistent 2D description of angular momentum and heat transport inside partly convective, rotating stars. P. Lesaffre and K. Chitre are revisiting and improving ideas dating back to the late 60's (Gough 1968) to predict the degree of anisotropy of local fluid motions, and the 2D fluxes of heat and angular momentum, with only one free parameter (the mixing length). Their prescription will be validated on 3D simulations of turbulence in rotating and shearing boxes, and extended to the magnetic case, for introduction in 2D axisymmetric stellar evolution codes.

Another recent puzzle is the wide range of field topologies in fast rotating low-mass stars, from dipolar to strongly multipolar, revealed by spectro-polarimetric observations (Donati & Landstreet 2009). M. Schrinner (ENS), L. Petitdemange, and E. Dormy (IPGP) showed that this behavior might be due to a bistable dynamo regime at low Rossby number. L. Petitdemange is codirecting a new Ph.D. thesis (R. Raynaud) with E. Dormy to verify if this result remains valid in a compressible anelastic case. Oscillating dynamos with a theta-dependent temperature will also be modelled to try and explain the sunspot migration sense (towards the equator) observed in the Sun, which is in opposite sense to that predicted by all current solar dynamo models.

### 3.5.2. Microscopic transport: radiation-matter interaction

*Delahaye, Zeippen, Sahal-Brechot*

The current improvement of observational data on stellar parameters, including precise spectroscopy, astrometry, interferometry and asteroseismology, is requiring a drastic improvement in stellar models. High-precision calculations of atomic energies and opacities for elements of astrophysical or laboratory interest will continue. We will improve accuracy by including 2-body terms, and compare with experimental measurements at LULI (collab. S. Turck-Chièze, CEA/IRFU). The treatment of radiative diffusion will be refined and new routines with updated atomic data included in the stellar rotational evolution code YREC, to improve predictions of solar/stellar parameters. With our Tunisian and Serbian partners, our numerical code for Stark broadening *ab initio* calculations will be generalized to complex atoms requested for stellar atmosphere models (O II and C I for hot DQ white dwarfs; B IV, Si II, Cr II and Cr VI etc). The results will enter the STARK-B database. An online version of the code is also planned.

# 4. Pole 3: Molecules in the Universe

**Thematic Pole 3**

*Are committed to Pole 3 research project after 2014 :*

*19 research and teaching permanent staff incl. 1 emeritus : C. Balança, M. Bertin, C. Boursier, H. Chaabouni, V. Cobut, F. Dayou, M.-L. Dubernet, F. Dulieu, J.-H. Fillion, M. Glass-Maujean, C. Janssen, X. Michaut, A. Moudens, L. Philippe, A. Spielfiedel, L. Tchang-Brillet (50%), Y. Te, A.-M. Vasserot, T. Zanon*

*1 long term research and teaching non permanent staff: E. Congiu.*

*6 PhD students having already started :O. Denis-Alpizar, M. Doronin, L. Gavilan, H. Lemaître, M. Minissale, I. Oueslati. Plus a number of PhD students and postdocs to be hired for the next period,*

*and 9 technicians and engineers : S. Baouche, C. Blaess (20%), N. Champion (20%), H. Elandaloussi, P. Jeseck, F. Lachèvre (50%), E. Somson (50%), P. Marie-Jeanne, C. Rouillé*

## *4.1. Scientific originality and strategic evolution*

Molecules, ubiquitous in our atmosphere and in space, are providing powerful tools for probing the physics and chemistry of many different environments. They provide important clues for major scientific objectives such as climatology, planetology, star and planet formation and the question of the origin of life. The analysis of molecular radiation under various extreme conditions requires nowadays a high level of knowledge in *molecular science* which has to support a wealth of observational data arising from new generations of telescopes, satellites and probes. The Thematic Pole “Molecules in the Universe” therefore seeks to push forward the current theoretical and experimental limits in order (1) to obtain *fundamental molecular parameters* with high degree of accuracy that are essential for probing and modelling complex media and (2) to understand and to predict an increasing number of unknown molecular processes that are involved in the evolution of matter in physical conditions specific to space and other environments.

This Pole brings together leading research groups in quantum physics/chemistry, low temperature physics, chemical physics as well as surface science researchers. It includes complementary theoretical and experimental researchers from different sites of LERMA and LPMAA, who have already established links, and who are very strongly involved in educational programmes of their universities.

The Pole aims at playing a major role at the interface between molecular and Astrophysics & Atmospheric sciences, being on one side fully invested in fundamental molecular and chemical physics communities but on the other side tightly connected to Astrophysical and Atmospheric research themes. This wide range of expertise and long standing experience in interdisciplinary research is an asset within LERMA² that should enhance the emergence of novel collaborative projects in particular with Pole 2 and Pole 4 (observations, media modelling, remote sensing and instrumental developments). Interactions with Pole 2 are of major interest to motivate new laboratory studies and to provide new ideas for observations

(ALMA, IRAM-NOEMA, Herschel, …).

Such an interdisciplinary group is rare in the same laboratory and will be both very competitive at international level and highly attractive for PhD students and Post-docs. Inter-disciplinary projects for PhD students (observational/laboratory/instrumentation) will be proposed. Pole 3 is naturally involved in molecular data-bases at different levels: HITRAN, BASECOL, SESAM, VAMDC and has a strong connection to the Support Pole.

Pole 3 is organized in 4 themes. Theme 1 deals with experimental studies of gas-surface interactions concerning heterogeneous chemistry and photon induced processes. Theme 2 addresses theoretical calculations and methodology developments concerning gas-phase processes, that will lead in the future to surface science theoretical studies. Theme 3 groups different technological approaches in order to study processes tightly linked to some molecular anomalies i.e. isotopic anomalies and out-of-equilibrium *ortho-para* ratios. Theme 4 is focused on reaching very high accuracy for spectroscopic parameters and sensitive detection of molecular compounds.

One of the strengths of Pole 3 is to develop sophisticated experiments and calculations to overcome the complexity of molecular systems and their interactions. The newly formed Pole 3 presents competitive capabilities, with relatively young permanent researchers, but not enough full-time researchers to ensure constant and high productivity. Most higher rank scientists of our present laboratories will have retired before 2014, which will imply that the younger scientists will have additional responsibilities, still reducing their available time. New research positions will be quickly needed, in order to fully develop the projects presented These weaknesses have to be progressively corrected in supporting the projects in all 4 themes presented below.

## 4.2. Gas-surface interactions

*Bertin, Chaabouni, Cobut, Congiu, Dayou, Dulieu, Fillion, Jeseck, Michaut, Moudens, Philippe, Spielfeidel*

This theme addresses the cycling role of dust in the chemical evolution of the Universe from the dying stars to the interstellar medium and the construction of new stars and planetary systems. Science developed within this theme focuses on the formation and destruction of molecules on grains surfaces at very low temperatures, in the context of puzzling questions about the origins of complex organic molecules in cold regions of the interstellar medium. Our project is built upon complementary expertise in heterogeneous chemistry (Dulieu and colleagues, 1,6 FTE), photon-induced processes (Fillion and colleagues, 2,6 FTE). It is supported by a shared-expertise in surface-science with the developments in the last 8 years of two of the most performing experiments (FORMOLISM, SPICES) in the very competitive field of **solid-state astrochemistry**. The science will develop with collaborations formed during the last years with other European leaders in laboratory astrophysics (Research Networks "LASSIE"- ITN-FP7-2008, Chem-ICE-Try-FP7-2013) and multiple financial supports (Labex UPMC-Michem, INSU-PCMI, Ile-de-France-DIM-ACAV, UPMC-Platform-ASTROLAB).

**The first major part concerns heterogeneous reactions** (led by Dulieu) with H, N, C and O atoms and molecular radicals on cold surfaces (silicates, carbonaceous surfaces, icy layers using FORMOLISM and soon VENUS set-ups). This part is supported by important technological optimization in atoms/molecular beams production and control that are under progress (BETSI set-up). A first axis concerns the chemistry on carbonaceous surfaces (PAHs, Graphite, amorphous carbon) interesting for diffuse ISM. Accent will be put on the interactions of H and O on well-defined surfaces (graphite/graphene) and comparison with STM experiments (collaboration Pr Liv Hornekaer Aarhus University (DK)). A second axis is dedicated to the molecular complexity that can be reached by heterogeneous chemistry on ices without addition of external energy (collaboration Catania University and Leiden Observatory started within LASSIE network). Acids (HCOOH) and amines ($NH_2OH$) have already been synthesized under astrophysically relevant conditions but the conditions and efficiencies for amino-acids synthesis remain to be found.

The second major part concerns **surface processes induced by VUV photons on ices** (led by Fillion) based on wavelength-dependent investigations that have been initiated since 2010 with the transportable SPICES set-up. We will pursue our detailed investigations of the photodesorption mechanisms on simple (pure or mixed) ices ($O_2$, $N_2$, CO, $H_2O$, $CO_2$ …) by using 2 complementary approaches (1) easy tunable synchrotron source (SOLEIL) and (2) VUV-laser selected wavelength sources that are under progress in the laboratory (P. Jeseck, see Sect. 4.6). Two laser pulses time correlated (VUV-UV) will be performed with the aims to enhance the understanding of primary steps in photon induced desorption. Besides a mass spectroscopic identification of products also their kinetic energy and, where possible, the population of internal rovibrational states will yield insight into the reaction. In this context, challenging determination of *ortho-para* ratio for relevant desorbing species will be attempted in links with the 3rd Theme (sect. 4.4). Dynamics in interstellar relevant ices induced by XUV pulses (fs) will be also undertaken using free electron laser (collaboration H Zacharias, Muenster).

A third part concerns the **determination of molecule-surface adsorption and diffusion energies on cold surfaces**, for a variety of key molecules in close collaboration between sub-groups (Fillion, Dulieu and colleagues). Such yet fundamental data are largely missing. In addition to be compulsory to the interpretation of all our experiments based on thermal desorption, this axis aims at contributing to fundamental data-bases compulsory for grain mantle formation simulation (collaboration with F. Pauzat, UPMC-LCT, P. Theule, PIIM-Marseille, and ANR project MIIA-Jan 2013). Special attention will be paid to characterize isomers and isotope shifts, as well as segregation processes or possible isotopic fractionation in link with the 3rd Theme.

**Guidelines and Evolution*:*** Experiments in the X-ray domain will be undertaken. Cosmic rays induced processes investigated by coupling our set-up on national facilities (GANIL, TANDEM…) will be considered at mid-term. Application to icy satellites around Jupiter, Saturn and to comets may also be also considered with more attention in the future. Long term evolution of Pole 3 will be to build a very strong theoretical and experimental surface science group.

## 4.3. Gas Phase Molecular processes

*Balança, Dayou, Dubernet-Tuckey, Spielfiedel, Tchang-Brillet.*

Science developed within this Theme aims at providing quantitative descriptions of gas phase collisional and reactive molecular processes relevant to probe and model astrophysical media. Our short and medium term project is built upon our expertise in the determination of potential energy surfaces for collisional (Spielfiedel) and reactive (Dayou) processes, upon our expertise on using collisional and developing reactive numerical codes (Dayou and

Balança) and upon our expertise on developing quantum and semi classical numerical codes for handling inelastic collisional processes (Dubernet). Our project is also built upon a strong collaborative theoretical and experimental network complementing the local expertise, as well as upon long-term collaborations with astrophysical groups allowing a useful match between the team's objectives and the needs expressed by the astrophysical community.

One part of the project (Dayou, Spielfiedel, Tchang-Brillet, 1 FTE) concerns theoretical investigations on still poorly known formation/destruction mechanisms of ICM key species. Our major investigation concerns the development of methodology for the study of **reactions involving large species**. Amongst gas-phase species, hydrocarbon species ($C_nH_m$) are particularly relevant since they are observed in a variety of astrophysical environments, ranging from diffuse to dense dark clouds and photon-dominated regions. The methodology to treat large systems will be further developed in the next *Quinquennal* leading steps by steps to organize and acquire full methodological procedures in order to investigate the field of reaction from isolated molecular clusters to surface science (see Sect. 4.6 Technology Program), 1 PhD student 100% co-supervised in Tunisia has already started on the gas phase aspects). In parallel we intend to investigate **low temperature reactivity of unstable radicals (OH, CH, CN) with atoms**, that are difficult to probe experimentally. For some systems comparisons are possible with experiments, such as the CRESU one in Rennes or the crossed-beam experiment in Bordeaux, allowing to test the highly accurate theoretical models that our team contributes to develop (Col. Rennes, Dijon, Bordeaux and Lille). Finally we will study **reactions involving UV field, such as the photo dissociation of SiO and the radiative association mechanism $C+H_2 \rightarrow CH_2+h\nu$** (Col. Lille). The large uncertainties on the rate coefficients of both processes are important issues for the modelling of chemistry in the diffuse ISM and in protostellar disks and jets

The second part of the project concerns collisional excitation processes involving molecules or atoms observed in non-LTE media such as interstellar medium, circumstellar, cometary or even stellar atmospheres. The demand for accurate rate coefficients is quite high with the upcoming ALMA facilities and the exploitation of HERSCHEL (HIFI) data. The team (Spielfiedel, Balança, Dayou, Dubernet, 1,5 FTE) has developed strong collaboration with theoretical groups and is one of the 4 leading French groups carrying out such studies, that will be pursued in order to tackle some new challenging issues *(i)* how to handle molecules with a large number of degrees of freedom such as **carbon chain species ($HC_n$), ($HC_n^-$)** which are key players for chemistry of C-containing species, line of work where the team will have a leadership (Spielfieldel, Balança, Dayou, Col. Madrid) *(ii)* how to characterize **collisional processes for high temperatures environments** where reactive paths should be considered for key species that probe warm and hot regions (Spielfiedel, Balança, Dayou, Col. Le Havre, Grenoble, Madrid) *(iii)* how to treat the dynamics of **strongly bounded cation molecules-$H_2$** collisional systems, such as $N_2H^+$-$H_2$ (Spielfieldel, Balança, Dayou, Col. Madrid, Grenoble) *(iv)* how to handle **excitation of molecules by water** for cometary applications and how treat the dynamics for the **excitation of low bending motion** (Dubernet, 1PhD in co-supervision with Bordeaux). Some of these studies will put a strain on the current methodologies. In particular the accurate determination of collisional rate coefficients with $H_2O$ has not been investigated yet and is a real challenge for the next generation of accurate collisional calculations, implying investigation of new methodologies, of more efficient algorithms for solving the Schrödinger equation and of using heavily parallel numerical codes. Finally the results of calculations will be disseminated through the BASECOL database that is now an international collaborative project.

In addition some current productive work will be continued concerning the excitation by H of atoms and atomic ions (Mg, Ca, O, and possibly Fe) of major interest for GAIA (Spielfiedel:

20% in collaboration with Marne-la-Vallée, St Petersburg, Uppsala).

**Guidelines and Evolution*:*** In the very long term, our objective is to extend our expertise towards investigation of reactions involving heterogeneous chemistry and photon-induced processes on surfaces (1st Theme). Therefore support towards that goal should be considered during the next *Quinquennal*.

## 4.4. Exotic isotopic and nuclear spin ratios.

*Bertin, Boursier, Chaabouni, Congiu, Dulieu, Elandaloussi , Fillion, Janssen, Jeseck, Marie-Jeanne, Michaut, Moudens, Philippe, Rouillé, Te, Zanon*

The science developed in this Theme is based on a phenomenological approach, which concerns the unusual, non-classic or not yet understood molecular signatures of multi-isotope or nuclear spin (*ortho/para*) ratios. Indeed, exotic multi-isotope ratios in molecules can be very sensitive tracers for specific molecular processes (eg $O_3$ formation). Similarly, *ortho-para* ratios likely provide information about the thermal and/or chemical history of matter, but the origin of out-of-equilibrium ratios may have multiple origins. Within this Theme, we investigate thermal and photochemical processes in the gas phase and on surfaces, by combining a multitude of complementary experimental setups developed within Pole 3 (Janssen, Michaut, Fillion, Dulieu and colleagues, 1,5 FTE).

The first part of our activities focuses on oxygen isotope anomalies in $O_3$, $H_2O$ and $CO_2$, which are presumably related to the gas phase or surface process of ozone formation, that lead to extremely large fractions (~ 10%) in both stable, heavy isotopes $^{17}O$ and $^{18}O$. This anomaly can be transferred to other molecules ($CO_2$, $H_2O$, …), possibly explaining the oxygen isotope inhomogeneity in the Solar System, and it is further assumed that thermal association reactions analogous to the O + $O_2$ reaction (such as O + CO → $CO_2$) can lead to an anomalous ratio in the oxygen isotopes. In order to better constrain the origin of these physico-chemical isotope anomalies, we will continue to study ozone formation and decomposition (photolytic and thermal) using a combined mass spectrometer and diode laser setup. With the evolution of the SIMCO instrument (LEFE-CHAT SIMCOII), which will add the triple oxygen isotope ($^{16}O$, $^{17}O$, $^{18}O$) measurement capability, we will measure the isotope composition of $CO_2$ from the thermal O+CO and the photochemical $O^1D$ + $CO_2$ reaction. Isotope effects on ices and relevant for the interstellar medium processes, in particular $O_3$ formation and the isotope transfer from $O_3$ to $H_2O$ will be studied with the FORMOLISM set-up. In the same time, fractionation processes involving oxygen isotopes will be investigated by irradiating $O_2$ ices (10 K) with VUV photons and monitoring surface reactions leading to $O_3$.

The second part concerns spin-enriched molecular samples preparations and their evolution in solid state at low temperature. Our major objective is to find experimental conditions that can produce out-of-equilibrium *ortho/para* ratios in the laboratory. We first focus on techniques that may produce enriched samples: (1) differential absorption column or optical pumping for gas phase sample initiated within the ANR-GASOSPIN project (2) molecular magnetic/electric deflection techniques (new collaborations with G. Alexandrowicz at Technion-Israel Institute of Technology and P. Ayotte at Univ. Sherbrook-Canada). The expertise (X. Michaut) developed in LPMAA during recent years will allow the characterization of the different nuclear spin states trapped in rare-gas matrices and to monitor the re-equilibration dynamics of the system ($H_2O$, $CH_4$ and $NH_3$) at low temperature. A second axis will concern nuclear spin equilibration dynamics of $CH_4$ and $H_2O$ at gas-ice interface at very low temperatures probed by FTIR in extremely low vapor and temperature controlled cells (COSPINU). Other experimental investigations will be devoted to surface processes. Firstly, we need to investigate physical effects. It will be done by probing the nuclear spin conversion dynamics of $H_2$ physisorbed on cold surfaces (graphite, molecular ices). The specific role of the photodesorption step will be studied, especially with $H_2O$, in direct link with the 1st Theme (SPICES, Laser UV-VUV experiments). Secondly, we also want to elucidate the crucial role of heterogeneous chemistry (FORMOLISM). Again OPRs in $H_2O$, after formation from H and O atoms reactivity on cold surfaces will be primordial, complementary to the above experiments.

## *4.5. Molecular parameters for planetary, terrestrial atmospheres and ISM*

*Blaess, Boursier, Champion, Elandaloussi, Glass, Janssen, Jeseck, Marie-Jeanne, Rouillé, Tchang-Brillet, Té, Zanon*

Reliable and coherent spectroscopic parameters of high quality are of an ever-increasing concern in many areas of research and society. In the framework of the community needs for improved spectral data on $O_3$, $CO_2$, $H_2O$ for actual and future satellite based climate (GOSAT, OCO-II, ACCURATE etc.) and space missions (JUICE), the spectroscopic properties of greenhouse gases, their isotopes and organic compounds will be studied within this science Theme.

Based on our competences in absolute precision spectroscopic measurements (Janssen), IR molecular spectroscopy (Boursier), laser spectroscopy and optics (Zanon, Elandaloussi), interferometry, and FTIR spectroscopy (Té) and instrumental development (Jeseck), we intend to develop a **molecular metrology** program for providing accurate, coherent and traceable spectroscopic parameters for atmospheric, planetary and astrophysical research. This comprises the development of **new technologies, absolute measurements** of spectroscopic parameters from the VUV to the Far-IR and inter-wavelength comparisons as well as **instrument intercomparisons** and **atmospheric measurements**.

For absolute **absorption spectroscopy measurements** in the IR, two major technical developments are planned for the next five years (Zanon, Elandaloussi, Janssen, 1 FTE): The development of new laser sources (ECQCL) micron range (acquisitions currently under way) and the long term development of a laser stabilization scheme based on frequency combs within the French EQUIPEX REFIMEVE+/FIRST-TF project. These technological improvements leading to an increased spectral resolution and absolute frequency calibration will be particularly beneficial for one of the project main goals: **Improving absolute spectral parameters so that isotope processes can be studied by absolute methods (remote sensing and laboratory)**. Starting with ozone isotopes in the framework of national (Labex Michem) and international collaborations (ISOZONE), we (Janssen, Zanon, Boursier, Elandaloussi, Té, Jeseck, 1,8 FTE) envisage the study of line parameters (positions, intensities, profile and broadening) of isotopic compounds ($O_3$, $H_2O$ and $CO_2$). This activity will greatly benefit from Pole 4 expertise in heterodyne systems and mm/sub-mm sources, because FIR-IR inter-comparison will allow absolute calibration of ozone isotopomers, which are difficult to assess otherwise. Future IR-FIR/sub-mm comparisons and studies for planetary research will be defined during the preparation of the JUICE mission (co-I SWI/JUICE Janssen).

In the VUV domain, analysis of very complex absorption and emission spectra of small molecules ($H_2$, $D_2$, HD) initiated in the previous period will be continued, and possibly new investigations of excited molecular states (high resolution spectra of $C_2$, CH or SiO in relation with theoretical studies of photodissociation (Glass, Tchang-Brillet, Champion, 0,8 FTE).

Another goal is the **development and improvement of spectroscopic techniques** for the **measurement of reactive and non-reactive atmospheric compounds (**Zanon, Jeseck, Té, 1,8 FTE**)**. Based on recent advances on frequency calibration, the SIMCO instrument will be improved to provide mass spectrometer accuracy within LEFE CHAT project SIMCO II . The FTS QualAir is about to join the international TCCON network to form a super site with the FTS at Trainou (Orléans). This activity involves the development of new reference cells and improvement of the retrieval schemes. SIMCO and FTS QualAir will be involved in inter-comparison campaigns with national and international partners (LSCE, IUP Bremen) to assess instrument reliability and complementarity of in-situ instruments and (fixed and mobile) remote sensing methods.

The measurement of short-lived (~ day) atmospheric species in the ppb range is challenging. Open path spectroscopic techniques provide a promising alternative as compared to non-spectroscopic techniques (PTRMS), because they are extremely selective and non-destructive. Within the framework of ANR MOCA-PRO, a long path configuration of the QualAir FTS for the measurement of atmospheric COVs for pollution studies is planned. This development requires new laboratory and multi-spectral spectroscopic studies of these compounds in order to reduce the yet very large uncertainties in spectroscopic data and to consolidate with spectroscopic methods operating in other spectral regions. In addition, the complementary approaches between laboratory and remote sensing experiments are extremely fruitful and attractive for the training of students, in particular PhDs.

**Guidelines and Evolution*:*** We expect that our implication in the JUICE mission will impact the orientation of our activities, strengthening links between Poles 3 and 4.

## *4.6. Technology program*

### 4.6.1. Ultra-high spectral resolution spectroscopy

Standard spectroscopic techniques (FTIR, Solid state lasers, etc.) hardly provide high enough resolution and accuracies for absolute isotope studies or for the next generation of satellite based climate observatories. With the advent of frequency comb technologies and ultra precise frequency standards, we plan to establish new spectroscopic techniques within the framework of national and local research structures of excellence (EQUIPEX REFIMEVE+/LABEX FIRST-TF/platform TF UPMC). This, together with our expertise on gas handling and the multitude of complementary spectroscopic instruments will lead to significant improvement of spectral parameters.

### 4.6.2. Atomic and molecular beams for heterogeneous chemistry

The high degree of control of atomic and molecular beams is a key strength of *FORMOLISM*. The development of new sources will open up the possibility to study multitude of yet unexplored surface reactions. Very stable and pure H and O beams have already allowed the studies of a large number of reactions. Implementation of N source is in progress, hydrogenated radicals source (OH, NH, CH) need now to be developed. Operating yields, quantitative flux control are crucial. We will thus develop a dedicated platform BETSI for testing, optimizing and characterizing atomic and radical beams, without sacrificing scientific production on VENUS and FORMOLISM set-ups.

### 4.6.3. VUV LASER

VUV photons used to irradiate cold samples will be generated by frequency tripling the output of a tunable laser (dye-laser pumped by YAG) in rare gases (Xe, Kr, Ar). A first scheme based on a closed cell tripling chamber coupled by an intermediate LIF window to a second chamber for fundamental/harmonic separation (rotating prism) will be built to cover the 110-150 nm wavelength range. A second scheme without any window will be designed to cover EUV range (below 110 nm), implying differentially-pumped chambers, a supersonic jet expansion for non-linear effect and dispersive grating. This equipment will strengthen our activity in Themes 1 and 3, complementary to synchrotron radiation on which beam-time allocation is very limited (about 5-8 days per year).

### *4.6.4. Development of special absorption cells and reference materials*

Special gas cells find widespread application for calibration purposes: on-board satellite instruments, for inter-comparison and calibration within international observation networks, and as calibration cells for laboratory spectroscopy. Based on past experience on the conception and characterization of reference cells for satellite missions (IASI, SWIFT), of cells for molecular spectroscopy (collisionally cooled Herriott cell, inert crossed beam cell) as well as based on our broad range of instruments (mass spectrometers, ultra high resolution IR lasers, FTIR instruments, precision temperature and pressure sensors) for the preparation and quantitative characterization of (isotopic) gas mixtures, we will keep on developing special purpose cells for our research and third body partners. In particular, we plan to develop

- The next generation of reference and calibration cells for European scientific laboratories and institutes within the TCCON network
- Reference cells for industrial partners, such as those required for the next generation of FTS on-board satellite instruments
- Inert low temperature cells for laboratory spectroscopy of climate gases and planetary atmospheric compounds

### *4.6.5. Open path FTS*

The development of a completely new measurement configuration “Open-path FTS” is on the way. This configuration (part of the ANR proposal MOCA-PRO) strives to measure reactive species like VOCs based on an optical method, which has the potential to overcome some restrictions of the more standard methods (isobaric mass interference in PTRMS). The aim is to build a compact and mobile version in collaboration with industries.

### *4.6.6. Theoretical developments:*

Theoretical descriptions of molecular processes rest on electronic structure calculations followed by nuclear dynamics simulations. We plan to develop original approaches to handle properly long-range interactions between open-shell species, couplings between excited states for moderately high-dimensionality systems, and to treat chemical bonding and weak interactions on an equal footing. In each case, the underlying idea is to combine the necessary ingredients (energetics, structural or electric properties) that originate from different quantum chemistry approaches.

The case of high dimensionality systems related to grains chemistry deserves a particular attention, as it is the main project where we wish to develop expertise for new theoretical approaches allowing thorough comparison with experimental studies on grains.

According to the representation of the surface, from isolated molecular cluster, embedded cluster to periodic cells, quantum chemistry approaches of decreasing level of quality have to be employed. The central idea we plan to follow is to develop reduced dimensionality (RD) models with isolated clusters of increasing size to represent the grains. Such RD models have been used by our collaborator B. Kerkeni (LPMC, Tunis) to deal with large species for gas-phase reactions (e.g. H+methylamine $CH_3NH_2$, CPL, 438, 1, 2007) and the formation of $H_2$ on a graphene surface (ChemPhys, 338, 1, 2007). Within RD models, the large number of degrees of freedom is separated between active modes (at least the bonds being broken and formed) and spectator modes. Our team (A. Spielfiedel and F. Dayou) is currently gaining this additional expertise on RD through the PhD thesis of I. Oueslati co-supervised by B. Kerkeni. In our project, both this particular RD expertise and our own on highly accurate electronic structure calculations and reaction dynamics methodologies will be combined. Indeed, the few number of active modes considered allows the use of accurate quantum chemistry methods to construct the multi-dimensional potential energy surface, and state-of-the-art quantum dynamics methods can be employed to achieve a realistic description of the reactive process.

# 5. Pole 4: Instrumentation and Remote Sensing

***Are committed to Pole 4 project:***

*Teaching and Research staff : Defer, Encrenaz, Maestrini, Prigent, Viallefond, Wiedner*

***Engineers : Boussaha, Caillat, Coulais, Dauplay, Delorme, Féret, Gatilova, Jimenez, Krieg, Lefèvre, Moreau, Treuttel, Zwölf***

*PhD Students :Defrance, and future students*

## 5.1. The THz instrumentation group

LERMA THz instrumentation group has been involved in the building of space-borne or balloon-borne heterodyne instruments dedicated to astrophysics, planetology or the sciences of the atmosphere for several decades. The group has built its R&D activities to master the design, technology and characterization of devices, circuits or entire heterodyne instruments. The group chooses its R&D projects based on the necessity to keep increasing the operating frequency and the sensitivity of heterodyne instruments to explore the universe with unrivaled spectral resolution, hence, with unrivaled ability to understand the underlying physics of the images that the astronomers are able to get from their telescopes. As a matter of fact, LERMA THz instrumentation group has always worked at the frontier of electronics in terms of frequency and sensitivity: its program for the next five year period is to continue in this direction.

### 5.1.1. R&D for Instruments

For the period 2014-2018 LERMA THz instrumentation group will be involved in the building or the upgrading of the instrument CIDRE and on the design, fabrication and tests of the synthesizers of SWI-JUICE. The group will continue priority R&D programs dedicated to these instruments.

- **HEB mixers for CIDRE**. The priority activities of LERMA THz instrumentation group will concern the development and the delivery of the HEB mixer for the balloon-borne instrument CIDRE. The group will continue to improve the design and the fabrication process to get higher sensitivity and larger intermediate frequency bandwidth. Particular efforts will be made to maximize the coupling efficiency between the mixer and the LO signal at 2.5-2.7 THz provided by a Schottky diode frequency multiplier chain. Studies on the extension to multi-pixels will be carried out in parallel in order to provide a four-pixel mixer for the second step of CIDRE experiment.
- **Schottky diodes for SWI-JUICE, CIDRE and ISMAR**. LERMA and LPN will seek to improve the yield of the current Schottky process, and to add on-chip capacitors to its circuits. On-chip capacitors are important to bias the Schottky diodes and consequently increase the performances while bringing greater flexibility to the circuit topology. In the meantime, LERMA THz instrumentation group will further investigate novel topologies of Schottky mixers and frequency multipliers based on LPN Schottky diodes or diodes of other European groups. The instrumentation group will prepare the possible delivery of the entire 1.2 THz channel of SWI-JUICE and the delivery of a local oscillator at 2.5-2.7 THz for CIDRE.
- In addition, the technical group will continue to work in collaboration with the remote-sensing

group to foster the development of a 875 GHz Schottky receiver with its own device technology, as an addition to the ISMAR airborne demonstrator for Earth ice cloud characterization in the framework of the preparation of the next generation of operational meteorological satellites.

### 5.1.2. Longer-term R&D programs

LERMA THz instrumentation group will also have long-term R&D programs to prepare future THz heterodyne instruments like the Far-InfraRed Interferometer (FIRI) or the Russian deployable 12m THz space observatory MILLIMETRON. Some of these R&D programs will be in partnership with physics groups of the PSL Idex and will use its fabrication facilities.

- **Heterodyne receivers with HEB mixers.** To meet the requirements of future far-infrared space or ground-based observation missions, the R&D on HEB receivers will be undertaken with the aim of increasing observation frequency range and receiver sensitivity by theoretical and experimental studies on different mixer designs. HEB devices on thick and membrane substrates will be developed. Quasi-optical and waveguide RF coupling circuits will be studied.

  At the same time, as large imaging detector arrays will allow high mapping speed, fine details and large fields of view, the THz instrumentation group will actively look for and explore solutions for making high performance THz heterodyne camera.

  LERMA THz instrumentation group plans to develop, with the newly purchased sputtering machine, the process to produce ultra-thin NbN films which are until now supplied by a Russian company with a near-monopoly on such films. High quality films for THz HEB devices are expected and in-situ device fabrication process will be considered. While seeking to use THz sources based on frequency multipliers, LERMA will keep its R&D activity on QCLs for LOs.

- **Physical modeling of THz Schottky planar diodes.** The coupling of physics-based device modeling, 3D-modeling of the EM fields as well as the thermal effects inside the circuit is an active field of research aimed to improving design accuracy. LERMA THz instrumentation group is part of such research effort in the frame of an ongoing FP7-MIDAS R&D program that will end in May 2013. The group is seeking to continue this effort in partnership with LPN and IEF.

- **Integrated SIS receivers**. LERMA THz instrumentation group will restart its R&D program on integrated SIS receivers featuring an LO made with multi SIS junctions. The goal is to demonstrate a functional and optimized single-pixel receiver to be replicated to build a camera

- **Characterization of dielectrics at sub-millimeter wavelengths**. LERMA THz instrumentation group plans to continue its program on the measurement of the dielectric constant of materials similar to those found at the surface of Earth, planets, or comets. The group has recently upgraded its test equipment for higher operating frequency and sensitivity. A cryogenic chamber and sample holder will be developed for measuring different types of ice. This preliminary study will help define the outline of an R&D program that will extend the existing R&D on sands and rocks. The group will seek the collaboration of French groups working on ice at different wavelengths since manipulating such samples is delicate. The group will collaborate with Dr. Fei Wang who was affiliated with the lab for two years to work in part on this program.

### 5.1.3. Contribution to other programs

LERMA THz instrumentation group processes world-class test equipments that could be part of a so-called THz platform of the Région Ile de France. The R&D can also have applications outside its research field:

Far-Infrared molecular spectroscopy. LERMA THz instrumentation group has discussed with several French molecular spectroscopy groups, including Pole 3, on the possibility of using its expertise on THz heterodyne detection and its world-class test equipment for experiments in the far infrared. Of particular interest is the possibility to use the numerous frequency-agile electronic sources owned by LERMA THz instrumentation group around 0.4 THz, 0.5 THz, 0.6 THz, 0.75 THz, 1.4 THz and 2.7 THz. Another possibility is to use one of the HEB receivers at 1.4 THz or 2.7 THz with the THz synchrotron radiation produced by SOLEIL.

**Novel magnetic field detectors or filters**. During past experiments, LERMA THz instrumentation group found that its mathematical model of nonuniform Discretized Josephson Transmission Lines (DJTLs) operating in their static regime, could be used to design efficient magnetic detectors and magnetic filters such as Superconducting QUantum Interference Grating (SQUIGs) and Superconducting Quantum Interference Filters (SQIFs). This could allow enhancement of the sensitivity of SQUID-based magnetometers and most importantly could provide absolute H measurements. This founding could lead to a new R&D program in collaboration with physics group.

## *5.2. Earth and Planet Remote Sensing*

The activities for the next years will be based on the expertise gained during the past two decades, with the involvement in several international projects and satellite missions, for the characterization of atmospheric and surface properties of the Earth as well as of planets. New techniques will be explored in connection with both the hardware and software instrumentation groups, within the same Pole.

### 5.2.1. Earth atmospheric remote sensing

#### *a) A new technique for the meteorological community: the sub-millimeter wave radiometry*

One major activity will be the validation of the millimeter sub-millimeter wave radiometry for the characterization of ice clouds. Ice clouds are key variable in the energy budget of Earth and are still poorly described at global scale. Several theoretical studies have demonstrated that ice clouds can be detected and their properties quantified with passive millimeter–submillimeter radiometry. The recent decision by EUMETSAT to have such an instrument on board the next generation of European operational satellites (MetOp-NG) will boost research in this direction. We are already part of the few key leaders in this activity in Europe and we plan to strengthen our contribution, in close collaboration with our European colleagues. An airborne demonstrator is under construction in the UK (the International Sub-Millimeter Airborne Radiometer, ISMAR), and LERMA will be leading the software development for this instrument, as well as the data analysis. The major outcomes of this project will be the development of the algorithms for the cloud and rain characterization, and the refinement of the specifications of future missions, especially MetOp-NG.

#### *b) Combination of multi-satellite observations for a better description of the Earth atmosphere.*

Accurate estimation of the atmospheric profiles (temperature, water vapor, clouds, rain, snow) from satellite is very challenging, especially close to the Earth surface over land, and under convective situations. We will keep exploiting the synergy of multi-satellite observations, from the visible to the microwave, both using active and passive modes, first to gain understanding in the physical processes, second to provide atmospheric retrieval with improved accuracy. For instance, estimation of snowfall at global scale is still very problematic. The complexity of the microphysical properties of snow makes it very difficult to simulate the radiative behavior of snow in the microwave. Using both active and passive observations over a large range of frequencies helps constrain the problem. We initiated some work in this direction and we plan to continue over the next years, in collaboration with the Global Precipitation Monitoring (GPM) team. Our team has a long experience in the analysis of the scattering signatures of clouds, in the microwaves, and we evidenced different ice particle habits, thanks to polarized scattering information. The French-Indian mission Megha-Tropique has been successfully launched, and provides for the first time polarized microwave observations up to 160 GHz. We just started the analysis of these observations, in order to better characterize the ice microphysics, especially in convective clouds. This work, in close collaboration with cloud modelers (LA) will help constrain the representation of the cloud microphysics in current atmospheric models, improve their description in radiative transfer codes, and better describe the regional, seasonal and diurnal variability of cloud and atmospheric properties. Synergy of space-based and ground-based – lightning, radar - instruments will also be explored for a better exploitation of available data stream in preparation for future missions, in support of field experiments (such as HYMEX) and for operational applications. More activities on sub-millimeter wave radiometry are currently underway, in collaboration with the technical group, such as the exploration of the potential of hyperspectral microwave measurements for a better characterization of Earth atmosphere. Interactions with Pole 2 scientists are underway to share expertise on multi-spectral analysis. Finally the retrieval techniques as well as the analysis methodologies are applicable to other targets such as planets and comets, offering the possibility to interact with teams involved in planetary exploration.

#### *c) Contribution to astronomical observations.*

The expertise of the group in atmospheric analysis can serve the astronomy community. Development and operation of a cloud monitoring instrument at ALMA and/or NOEMA site have already been discussed, in collaboration with the technical group and with Pole 2, in order to improve ALMA / NOEMA operations under high cloud operation. Investigation of MIRO observations during the three Earth fly-bys of the ROSETTA spacecraft is a unique opportunity to test MIRO instrumentation. The expertise of LERMA in atmospheric retrievals helps characterize the astronomical observations, and an efficient collaboration with LESIA has been put in place. Other astronomy-atmospheric application plans the use of LOFAR for the detection and characterization of the lightning flashes in Earth thunderstorms and for an inter-operation with the up-coming Meteosat Third Generation Lightning Imager (MTG-LI, optical sensor), designed to monitor in real time the lightning activity from Earth geostationary orbit.

### 5.2.2. Characterizing the surface of planets and comets

#### *a) Improved hydrological characterization of the land surface at global scale.*

Our group is deeply involved in different international projects related to land surface characterizations with satellite observations. These projects will continue over the next years, and we intend to pursue our efforts on these activities. The recent launch of the SMOS (Soil Moisture and Ocean Salinity) satellite (interferometer at 1.4GHz) provides the community with the first observations directly dedicated to the soil moisture. Our group started to analyze the new data and to combine them with the other available satellite observations for an improved hydrological characterization of the land surface. We are also involved in the NASA/CNES SWOT (Surface Water and Ocean Topography) mission and we will invest in the preparation of the analysis of these observations, thanks to the expertise we acquired in the wetland detection and characterization. We belong to the Science Advisory Group of the French-German MERLIN satellite project (phase B at CNES). Our role will be to provide this community with land surface information to optimize the retrieval of methane concentration.

#### *b) Production of long-time record of global land surface parameters.*

The land surface products we develop and distribute are used by the climate community, and require long time series. We will continue the production of these variables, up to current time, adapting the processing to the new satellite missions. We will also keep working on the analyses of the inter-annual variability of these time series, and on the potential trends, in collaboration with the climate community. Contributions include the production of dynamical surface water extent and land surface microwave emissivities. We are also co-leaders of the GEWEX LandFlux activity that will produce reference land surface turbulent fluxes from satellite observations, within the next years. Part of these studies are encouraged and supported by ESA.

#### c) Closing the Earth water and energy budget with satellite observations.

There is now a broad variety of global satellite products describing the Earth water and energy budget. We participated to the development or the evaluation of several of them. The scientific issue is now to close the Earth water budget, and to predict any change in the hydrological cycle, related to a warming climate and to demographic pressure. Are the satellite-derived datasets accurate enough to diagnose any change in the hydrological cycle? We plan to contribute to analyze this problem, and to keep working on the development of the accurate satellite retrieval of surface variables toward this aim.

#### d) Strengthening our collaboration with the land surface modeling community.

In the next years, we want to strengthen our collaboration with the land surface modeling community, in order to optimize the use of satellite observations for model evaluation and climate analysis. The two communities acknowledge a need for more interaction, but this is not an easy task, as the two communities (model and remote sensing) have very different approaches. A dialog has started with the LMD (IPSL) and with foreign labs (e.g., CEH, NASA), but this effort is to be consolidated, possibly through joint projects.

#### e) Planets and comets.

The Cassini mission has been extended by 8 years, after the 2009 equinox. The wealth of data already obtained about Titan evidenced the presence of a large variety of environments (dunes, lakes, seas, craters). Some observations such as the extreme flatness of lakes, or the sudden changes in lake levels are still not explained. The mission life extension will make it possible additional observations under different solar conditions and will help explain the physical behavior of the Saturne satellite. In the framework of the Rosetta mission, measurements of the dielectric properties of different comet-like material will continue, in collaboration with the technical group.

## 5.3. Software instrumental activity

The birth of physics as a modern science during the seventeenth century is related to the use of mathematical framework for describing the laws of nature. The mathematical ontology and its formalism accelerated the development of this science. Nowadays, with the rise of computer science and their massive diffusion, we have to face issues similar to those faced by physicist in seventeenth century: the computer-science formalisation of physics and the achievement of computer ontologies for physics. This is meanly the theme of the computer-science instrumental research of this Pole 4.

This activity will keep focusing on three items (closely linked):

- Formalisation of the reality through generic data models. Thus, the resulting models will be used to rationalize and perpetuate the observational data (e.g. coming from instruments such as Alma, Gaia or SKA) or results from simulations.
- Formal methods for data understanding. This axis is dedicated to formal models of a priori knowledge (through ontologies and description logics) in order to guide the analysis and the extraction of the semantics of data.
- Interoperability algorithms and solutions. This axis focuses on building a real physical interoperability (not only in a computer science sense), based on the physical nature of the handled object (its physical meaning, its unit and precision, and the range of admissible

values). Naturally this axis uses inputs from the two previous. The tools developed in this context will permit straight and automatic interoperability between the online computation/visualisation services and the theoretical/observational databases.

This kind of formalism, resulting by combining these three axes, will make it easy to achieve (otherwise complex) processing, such as:

- Conversions and/or inter-calibration required for working with heterogeneous data (by structure and format).
- Discovery, search, extraction, visualisation and post-processing of a particular data among several Terabytes of heterogeneous data.

# 6. Transverse Scientific Services

## *6.1. National observing services*

LERMA² will carry on LERMA's contributions to the *Services d'Observation* nationally managed by INSU in various ways. These services are carried out by astronomers, as mandatory duties of the special CNAP body of civil servants, and staffed by support personal dedicated by the lab to these tasks, as well as voluntary contributions by university and CNRS staff.

### 6.1.1. Services AA/SO2/SO3

LERMA has acquired a strong expertise in hardware and software instrumentation based on high frequency heterodyne receivers. Short term (to end 2014) contributions to the ALMA and SKA projects are ongoing, longer term proposals are being prepared, both on hardware and software developments. On hardware side, the current R&D outcomes on advanced local oscillator sources and heterodyne cameras open promising solutions for the next generation focal plane instruments of NOEMA and ALMA. The development of very high frequency detectors led to proposing the CIDRE balloon project, preparing for a large project in a much remote future (heterodyne FIRI). On software side original contributions will be pursued on data models and observatory archive architecture, with applications to ALMA and SKA. In addition LERMA, co-founding laboratory of IRAM, and forefront promoter of the Herschel and ALMA major projects will continue to support their operations by sending a few of its staff members into these observatories, and by educating young scientists who will later work there.

#### *a) Project for developing an ALMA archive mining service*

LERMA² will continue its involvement into the Alma Regional Center in Grenoble and will propose additional scientific services related to ALMA. Indeed the science data produced by ALMA are systematically archived and they become public one year after their release from the observatory to the PIs. The ALMA project is developing a science archive (ASA) but its scope is limited given the complexity of the data.

In that context it is the proper time to develop science driven data mining tools especially to generate transversal scientific programmes by composing the native datasets produced by the telescope. Therefore it is proposed to develop what is necessary to process and analyse jointly data obtained in different experimental setups, this in home environments of the users to allow high interactivity This development will capitalize on the fact that the Science Data Model is natively a database based on an open technology to make the interface with the processing units.

This project, a service proposed by LERMA² in prolongation to its involvement for the ALMA construction, is motivated to extend its expertise in radio interferometry and to give the users a convivial and efficient environment maximizing the scientific return of the ALMA data.

#### b) SKA data model and data handling system

The data model developed by LERMA for ALMA has been adopted by NRAO for the E-VLA project, and is now proposed as the basis for SKA data management. A prototype implementation is currently being developed on the EMBRACE demonstrator for validation. Strong interest has been expressed within the international SKA community for the advanced concepts developed in support of this data model, which offers a natural support to the measurement equation and instrument calibration.

#### c) Signal processing

Expertise has also been developed on data processing of long wavelength direct detection instruments (from ISO onwards, and currently Planck). The plan is now to propose an expert contribution to the SAFARI far infrared spectro-imager onboard SPICA.

### 6.1.2. Services AA/SO5

Diffusion of atomic and molecular data and of theoretical results produced by state-of-the art codes have always been a strong activity in LERMA. Indeed, an efficient scientific return of large instruments is only possible if such services are provided to the community. These activities will be strongly enhanced in the next few years thanks to the expertise gained in the recent years at LERMA and because more and more scientists of the laboratory want to participate to these activities. Moreover, LERMA2 will get new international responsabilities on these activities with the arrival in the laboratory of the P.I. of the VAMDC project (from LPMAA) and the chair of VO-Theory at the IVOA (from LUTH). Both services have been proposed for « labellisation » to the CSAA.

#### a) Service « Atomic and Molecular Data Diffusion/VAMDC »

VAMDC activities (http://vamdc.eu, LPMAA-AP-13) at Paris Observatory will be mainly located in LERMA2 and cover atomic and molecular databases developments and maintenance within VAMDC : SESAM (http://sesam.obspm.fr), TipTopBase, BASECOL (http://basecol.obspm.fr), Stark-B (http://starb.obspm.fr), the development/maintenance of some of the VAMDC standards (http://vamdc.eu/standards) and software (http://vamdc.eu/software) as well as the coordination of the national «Pôle Thématique F-VAMDC » and the coordination of whole International VAMDC consortium. As an heritage from LPMAA, LERMA2 will maintain the portal (http://portal.vamdc.eu) LPMAA-AP 14), continue to upgrade the tools developed such as TAPValidator, Node Software in Java (LPMAA-AP-15) and SPECTCOL (LPMAA-AP-12) and develop other tools in relation with astrophysical user needs. LERMA2 will work closely with the DIO in order to ensure that DIO continues to maintain its activity in VAMDC : monitoring of the infrastructure, replication of services, support system and grid access. Other activities will range from outreach to political and policy issues within the consortium. A new european project, SUP@VAMDC, running from Decembre 2012 to Decembre 2014, coordinated by M.L. Dubernet, will pave the way to extension of VAMDC to other continents and databases and to building a sustainable, open access international consortium. It is hoped that a permanent position could be assigned to support LERMA2's leadership in VAMDC.

#### b) Service « ISM/JET Platform and VO-Theory »

LERMA is one of the main contributors at IVOA for the development of standards and software architectures to publish theoretical data and to provide online state-of-the-art numerical codes. PDRDB (http://pdr.obspm.fr) and Starformat (http://starformat.obspm.fr) are the two theoretical services used at IVOA to validate VO-Theory standards. These R&D activities gave to the laboratory a unique expertise among french astrophysical laboratories (with CDS) on some new I.T. technologies required to provide access to complex data : management of mass of metadata, web semantics, machine learning, Grid computing. These technologies are used to develop GALMER (http://galmer.obspm.fr), STARFORMAT (http://starformat.obspm.fr) and PDRDB (http://pdr.obspm.fr). The technical expertise gained in the recent years allow us to gather some of our services to begin the development of a platform providing all the types of numerical models required to interpret observations of the interstellar medium with the new generation of instruments (Herschel, ALMA, Noema, Gaïa, ...). This platform, developed in partnership with CEA/SAP, IAS and other french and international teams, will give access to MHD simulations of interstellar gas and jets, models of the physics and chemistry of interstellar gas (PDR, chocs, radiative transfer,turbulence), models of the physics of grains, etc. Databases and online codes will be fully interoperable with the Virtual Observatory and VAMDC.

### 6.1.3. Service OA : « Global Surface Parameters from Multi-Satellites (GSPMS) »

Unique databases of global land surface parameters derived from multi-satellite observations have been developed at LERMA by the remote sensing group. They cover long time series (up to 15 years) and are of interest for land surface analysis as well as to for atmospheric studies. These land surface variables include atlases of microwave land surface emissivities (e.g. for the operational assimilation of satellite microwave observations over land), flood dynamics (e.g. for hydrological studies, methane emission analysis), aerodynamic roughness lengths (for aerosol modelling). They are widely distributed to the national and international communities (more than 50 registered users for some products), are used in a large number of publications, are adopted in climate models (Orchidée, ISBA, MPI, NASA/GISS), and are integrated in community radiative transfer models (EU RTTOV, USA CRTM).

A “service d’observations (SOERE)” has been proposed recently to maintain and distribute these valuable data sets, to continue the production of the time series, to perform quality control on the outputs, and to adapt and improve the retrieval algorithms. It would require the hiring of a permanent research engineer.

## *6.2. Objectives of training through Research*

LERMA² contributes to a large variety of graduate training programs in several scientific domains including observation, theoretical and numerical astrophysics, experimental, theoretical and numerical molecular physics and plasma physics, remote sensing, instrumentation and electronics.

Our Project includes the reinforcement of on-going actions in order to improve the quality of the doctoral training, as well as the complementary professional training, in preparation to the future career of the laureates, whether academic or not. These actions include:

- proposing technical training in order to develop skills in computer science, electronics, optics, laser, ... as well as project management and management techniques. LERMA² will take initiatives as part of its life-long training program for the laboratory staff, and encourage graduate students to attend courses offered by the Doctoral Schools,

- Distribute a list of professional contacts outside of the academic environment,
- Organise communication events related to the scientific training policy,
- Encourage exchanges among students and post-docs within the poles, as welle as between poles and sites,
- offer 2 weeks internships in a different team to PhD students, every year.

## 6.3. *Teaching and Outreach*

LERMA² has a strong involvement in teaching physics, astrophysics, electronics at all University levels (see reports from LERMA and LPMAA) at *Université Pierre et Marie Curie*, *Université de Cergy-Pontoise*, *Observatorire de Paris* and *Ecole Normale Supérieure*. In addition the engineers from GEMO have teaching activities in various Engineering schools and technical departments of universities, with the plan to focus more of the effort in the engineering department of UPMC, where is is already very active. The overall teaching involvement will be further extended within the new PSL teaching infrastructure.

A new project under construction is the installation of a pedagogic observation platform on the refurbished UPMC roofs, equipped with of a radio antenna and small optical telescopes, aimed at practical trainings of physics and engineering students from Licence to Master Levels. The automatic radiotelescope is also integrated in the European « Hands-on Universe (HOU) » network, that aims at disseminating science/astrophysics into schools.

Another new project of LERMA² will be to establish a connection between the « (HOU) » project and the VAMDC Consortium that aims at disseminating atomic and molecular data produced in the research laboratories (SUP@VAMDC project, see section on Scientifc Services in the previous chapter).

## 6.4. Communication

External Communication will be aimed at different audiences: governing bodies, researchers, high education, schools, SMEs and citizens. The aim will be to present/represent the laboratory activities in order to increase the attractiveness and visibility of our teams, thus enabling the creation of new opportunities.

Internal communication will increase the sense of partnership across the sites and teams (pole), possibly creating new collaboration opportunities.

The foreseen actions will be a well-throught internal and external website, leaflets, organisation and participation to events, organisation of internal small meetings for students and post-docs, yearly scientific gatherings outside the usual premises.

# Part 3.
# Project implementation

# 1. Missions of the Technological Pole and Research Support

This Pole regroups all the technical and administrative staff – ITA and IATOS.

It is managed jointly by the technical director and the laboratory administrator.

## 1.1. Administrative support

The main mission of the administrative team are:

- assist the directors in managing the laboratory,
- support project leaders in proposal preparation,
- prepare and execute the budget, carry on expenses, follow-up contracts,
- manage human resources, follow up careers and life long learning,
- take care of general maintenance, and provide various logistic and secretarial services,
- interface with the central administrative services of the governing institutions (CNRS, Observatoire de Paris, ENS, UPMC and UCP),
- organise or provide assistance with various laboratory events: arrival and departure of personnal, students, interns and visitors, meetings, seminars, workshops and conferences, $LERMA^2$ days, celebrations.
- enhance communication and supervise laboratory internal and external websites

The current proposal for the administrative organisation (see Fig. 3.1.2) derives from the LERMA current organisation adding the competences of the LPMAA administrator. In 2013/2014 optimisation of financial and human resources administration will be carried out in order to cope with the retirements of 2 administrative assistants.

The communication and web sites activities are currently carried out by various people (administrative, engineering, research staff), are based on good will and represent an extra workload. Moreover we believe that more work is needed in order to achieve proper standards in the matter. However this extra workload will not be bearable by the remaining agents, if the administrative assistant of the ENS site is not not replaced when she retires at the beginning of 2014.

## 1.2. Technical support

- To support instrumental projects and R&D activities led within the scientific poles
- To provide general purpose support (computing and network administration, database software, mechanics, electronics,…) to the laboratory staff
- To facilitate the transverse activities between different sites and teams.

Most of the members of the technical staff are also members of the scientific poles, given the high level of expertise required to carry out their work in cutting edge fields. Nevertheless, a variable and negociable part of their time may be dedicated to support or expertise activities for other teams, in order to match the laboratory workload.

### 1.2.1. In-house Technical Facilities

#### a) *Commercial electronic and electromagnetic simulation software*

- Altium Designer, Microwave Studio CST, HFSS (High Frequency Simulation Software) ANSYS, ADS AGILENT are widely used, both for project and educational purposes
- Simulation results are correlated with experimental results
- Additional manpower needs are generally fulfilled by temporary staff positions.

#### b) *Cleanroom fabrication*

- Specific devices are fabricated in different technologies : SIS (Superconducting-Isulating-Superconducting) devices, HEB (Hot Electron Bolometer) devices, Schottky devices
- More general purpose circuits (substrate metallization,…) can be fabricated in the cleanroom
- A research engineer position is absolutely needed in **2013** to perpetuate the Terahertz Schottky devices fabrication activities (recruitment planned by Observatoire)

#### c) *Mounting technology*

- Means for mounting and wiring of microelectronic circuits and devices can be made available to the various teams
- No additional manpower requested.

#### d) *PA/QA (Product assurance/Quality assurance)*

- This function is no more available in the laboratory
- A shared manpower approach has been put in place at Observatoire de Paris, but not yet extended to LERMA
- Current projects are based on external temporary contracts.

#### e) *Mechanical Workshop*

- Mechanical activities are carried out at Cergy, at Observatoire de Paris and at UPMC. At each site the activities either are included in common workshops with other laboratories or are carried out in good collaboration with other labs workshops (UPMC). The competences cover computer-assisted design, mechanical manufacturing and an unique expertise on soldering at UPMC. No further support is required. At each site the technicians are perfectly trained to meet the specific needs and to produce high quality products.

#### f) *Electronic Workshop*

- Electronic workshop is involved in the experimental platforms at UPMC and more recently on the CIDRE project. Competences include analog and numeric electronics (computer-assisted design, simulation, board realization) applied to a wide range of experimental set ups. No further support is required.

### 1.2.2. Computing and Information Systems

The computing, information systems activities cover a wide range of competences:

#### a) System Administration

LERMA² is a multi-site laboratory where various devices need to be taken care of: personal computers, different communicating devices and in-house clusters (up to 1500 cores) on 3 sites. This requires both traditional system administration and the capability to address safely the integration of new technologies in our numerical environment. This triggers the need to replace the position of Mr Zidani in **2015**.

#### b) Numerical Simulation (High Performance Computing):

The 2020 challenge of exa scale computing requires a significant evolution of numerical codes: algorithms and adaptation of codes to new architecture. Currently some issues are handled by non-permanent staff; nevertheless to be at the forefront of international competition requires a long term strategy, that is the hiring of a permanent HPC engineer in **2014**.

#### c) Data Processing, Instrument Modelling:

The Signal Processing and data inversion competences, acquired for the past 4 years in Earth remote sensing, must absolutely be consolidated in **2013** in order to ensure the French leadership of Pole 4 in the scientific exploitation of the ICI instrument on board the EumetSat Polar System Second Generation (EPS-SG) satellites.

Both the Data Processing and the Instrument Modelling competences are vital for the implication of LERMA² in large astrophysical projects (ALMA, SKA, SPICA, FIRI, etc) and SO2 activities, the related activities being carried out by 3 senior research engineers. The retirement of two of them in 2016-17 should be anticipated in order to keep a strong task force, through the employment of one person in **2017**.

#### d) Software Development for scientific services ("Service d'Observation")

The Virtual Observatory Theory development is lead at international scale by LERMA². In order to keep the leadership in this ambitious project, and carry on fully consistent developments it is essential that the engineer in charge of the project architecture joins the laboratory with the project leader in **2014**.

VAMDC Infrastructure has been solely developed with the support of EU-FP7 and a project manager/chief software expert would be needed in order to sustain the developments made at Paris Observatory and in order to support French leadership in the VAMDC consortium. To be coherent with other laboratory priorities a position would be requested in **2016** only.

Research and Development in Computer Science is part of LERMA² activities at a modest level (see section 4.3 on Pole 4). It does not require further support.

### 1.2.3. Experimental Platforms

LERMA[2] has a strong technical experimental laboratory activity related to instrument design and development, instrument control (Labview, C, FPGA), laser and optical cavity, cryogenic and vacuum engineering, high resolution spectroscopy techniques from UV to infrared, lasers, interferometry, mass spectroscopy, and includes several experimental platforms listed below. The UPMC/Pole 3 activities are already supervised by 2 senior engineers, but lack of technical assistance in experimental physics; while the Cergy experimental platforms FORMOLISM and VENUS require a senior technical supervisor for design, calibration and supervision of the technical work. The experimental platforms of UPMC/Pole 3 requires a technical assistant who could as well be of assistance to the Laboratory of Plasmas Diagnostics of UPMC/Pole 2.

#### a) Surface chemistry for astrophysics (Cergy)

##### (i) FORMOLISM

is an ultra-high vacuum system operating since 2002. It includes 2 atomic and molecular beams (H, N, O, $H_2$, ...) aimed at cooled samples (6-300K). Mass spectrometry, laser and infra-red absorption spectroscopies are the analyzing tools.

##### (ii) VENUS

is an ultra-high vacuum chamber in development since 2012. It includes 5 beams with tunable fluxes, aimed at one target of the rotatable sample holder (4 different samples). Real time infra-red spectroscopy and mass spectroscopy are the analyzing tools.

#### b) Molecular laboratory astrophysics (Jussieu)

##### (i) SPICES

is an ultra-high vacuum system operating since 2010 and is designed to be entirely transportable. It includes a rotatable cooled sample holder (6-300K) coupled to mass spectrometry, laser and infra-red absorption spectroscopies. The system can be coupled to various photons sources (synchrotron, laser VUV beam lines).

##### (ii) COSPINU

is a high resolution Fourier-Transform Spectrometer (FTS) instrument operating since 2011 and coupled to an external close-cycle cryostat, for nuclear-spin conversion studies at very low temperatures (4-300 K).

#### c) Atmospheric spectroscopy

##### (i) QualAir *FTS*

is a very high spectral resolution (up to 0.0024 $cm^{-1}$) and very wide spectral range (from 233 nm to 22 µm) Fourier Transform spectrometer, operating since 2007. Associated with a sun-tracker, this instrument monitors the atmospheric species in and above Paris megacity. Due to its high resolution, it can be used for spectroscopic studies in gas cells.

##### (ii) Mobile FTS

is a Fourier transform spectrometer with a spectral resolution of 0.02 $cm^{-1}$ and a spectral coverage from 760 nm to 15 µm, operating since 1994. Coupled to a sun-tracker, the instrument provides remote sensing measurements of atmospheric constituents in the field.

**(iii) SIMCO**

is a transportable diode laser based absorption spectrometer for the measurement of the concentration and 13C isotope composition of atmospheric carbon dioxide, which is in operation since 2010.

### *d) Ultra-high resolution spectroscopy (Jussieu)*

**(i) TLSI**

Tuneable Laser Stabilized by Interferometry for the measurement of IR molecular spectra of stable molecules has a very high resolving power of 2 $10^7$ at 10 µm. Depending on the source laser, it can be operated in the 2 to 10 µm range and is currently prepared for operation with ECQCL (external cavity quantum cascade lasers) and stabilization by frequency comb techniques.

### *e) 10-meter spectrograph (Meudon)*

is a high resolution instrument for VUV (down to 195 Å) emission studies providing accurate wavelengths and linear intensity measurements. Investigations mainly concern electronic spectra of small molecules (Pole 3) and spectra of multicharged atomic ions for applications to stellar and solar atmospheres as well as for magnetic fusion plasmas (Pole 2).

### *f) Laboratory of Plasmas Diagnostics (Jussieu)*

is a unit preparing mobile sample cells and diagnostics instruments for plasmas studies using high power lasers and plasmas confinement systems.

# 2. Resources needed for the project implementation

The implementation of our project relies on the different types of resources that we may expect: human resources, financial resources, equipment and premises. The salaries of our permanent staff are paid by our governing institutions (*tutelles*): the CNRS contribution is still significant but tends to decrease in recent years. In addition to the recurring financing from the *tutelles*, which cover the basic running costs of the laboratory, but do not allow a significant financing of research projects since the drastic reduction of the recurring financial support from CNRS, investments, scientific travel, and non permanent staff rely on soft money obtained from various calls for projects from a number of national and european financing agencies.

## 2.1. National and International Projects and Contracts

As described in our scientific reports, our 4 Poles participate to *Investissements d'Avenir* projects. 6 *Laboratoires d'excellence* (LabEx meaning Outstanding laboratory or network project):

- the UPMC *Institut Lagrange de Paris (ILP) for Pole 1*,
- the UPMC *Plasmas à Paris* project (PLAS@PAR) led by LERMA² and the ENS *International Center for Fundamental Physics* (ICFP) for Pole 2,
- the UPMC *Multiscale Interactions in Chemistry* project (MIChem) and the CNRS *Facilities for Innovation, Research, Services, Training in Time & Frequency* network (FIRST-TF) led by SyRTE at Observatoire de Paris for Pole 3,
- and the Observatoire de Paris *Exploration des Systèmes Planétaires* project for Pole 4.

In addition LERMA² teams participate to 2 *Équipements d'excellence (EquipEx*, meaning approximately *Outstanding Equipment Project)* Equip@MESO dirigé par le GENCI *Grand Equipement National de Calcul Intensif*, and REFIMEVE+ led by Université Paris 13.

The 4 thematic poles also benefit from project based funding by :

- their hosting institutions (Observatoire de Paris, École Normale Supérieure, Université Pierre et Marie Curie and Université de Cergy-Pontoise)
- scientific programs supported by the regional Ile-de-France Council, especially the *Domain d'Intérêt Majeur* (DIM) *Astrophysique et Conditions d'Apparition de la Vie* (ACAV), and the heavy equipment SESAM program.
- French funding agencies (mainly ANR, national programs of CNRS: PCMI, PNCG, PNPS, PNP, and LEFE, and CNES)
- European agencies (mainly FP-EU, ESA, ESO)
- and occasionally US agencies (NASA and NOAA

LERMA² leads the *Microwave Remote Sensing of the Atmosphere* National coordination

(GDR stands for *Groupement de Recherche*), and contributes to the *Molecular Spectroscopy* (SPECMO) GDR, to the European Dynamo GDR (http://mhd.ens.fr/GDRE/), as well as to the research group ECOCLIM, submitted to PSL for extra funding.

The complex set of national sources for funding fundamental research in France has been successfully exploited by LERMA and LPMAA over recent years in combination with a few international grants and contracts, most of it for the PhD and postdoc funding, temporary technical support, research running costs and investments.

| Pole | LABEX | EQUIPEX | IDEX | Others |
|---|---|---|---|---|
| 1 | ILP | Equip@Meso | PSL, SUPER | ACAV, PNCG, CNES |
| 2 | Plas@Par, ENS-ICFP | Equip@Meso | PSL, SUPER | ACAV, CNES, PCMI, PNPS |
| 3 | MIChem, First-TF, IPSL | REFIMEVE+ | PSL, SUPER | ACAV, PCMI, PNP, LEFE-CHAT, UPMC Platforms |
| 4 | ESEP | | PSL, SUPER | LEFE, CNES, ESA, Industry |

In order to carry out our project during the 2014-2018 period, we need and intend to apply for the similar amounts of grant funding as in recent years, which amounted over the past 4 years to: 3.4 M€ for Pole 1, 1.6 M€ for Pole 2, 3.4 M€ for Pole 3 and 1.6 M€ for Pole 4 (annual average of 2.5 M€).

## 2.2. Research and teaching positions

The distribution of permanent research and teaching staff ages presently committed to the LERMA² project, and not retired at the beginning of the term is shown in the 2 figures below. While the overall age distribution is rather smooth, with a median in the mid forties, the differential distribution of CNRS vs University positions is striking, the latter being by far much younger. The Poles, on the contrary, show not much contrasted distributions, though the astrophysics teams have a significantly more senior members. As a matter of fact 10 of these seniors will have reached 65 before the end of 2018, representing about 20% of the total number. The list of the recruitments deemed necessary for the success of our ambitious project does not much exceed this number. In addition, recent departures, or departures

The positions listed below are needed to consolidate the expertises which are mandatory for the Lab to stay competitive in our leading research themes, taking moves and retirement of staff into account. The development of these expertises more and more relies on non-permanent staff: while it represents a significant investment, this development needs to be made profitable on the long-term, which is impossible with insufficient numbers of permanent staff members. Because the laboratory has very limited influence on the recruitment process, the needs are listed over the 2014-2018 period. Much more detailed hiring plans and priorities are yearly discussed with our governing institutions.

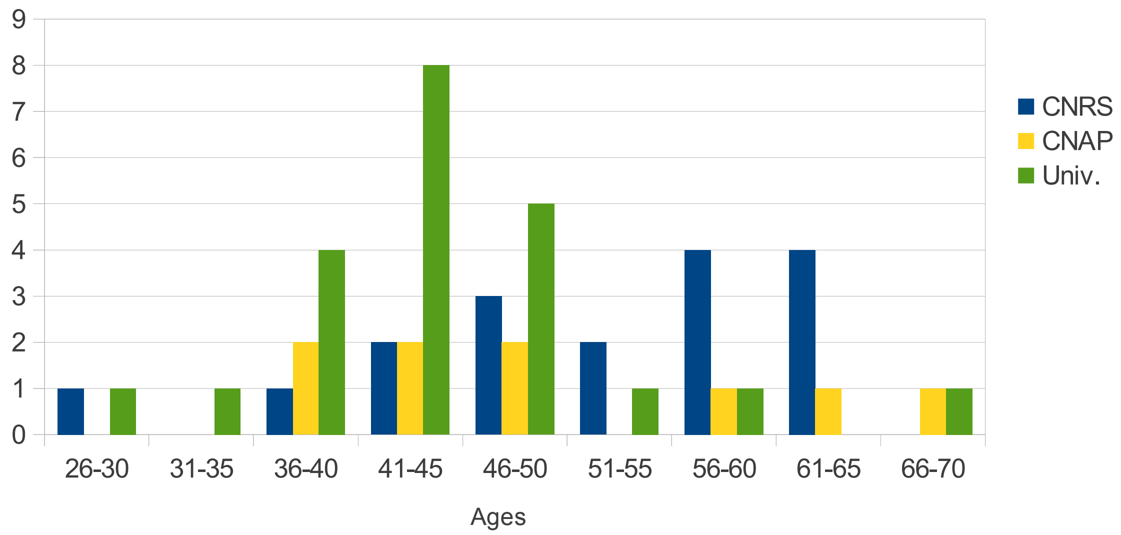


*Fig. 2.1: Age distribution per academic statute of the research and teaching permanent staff currently commited to the LERMA² project, as of January 1st 2014*

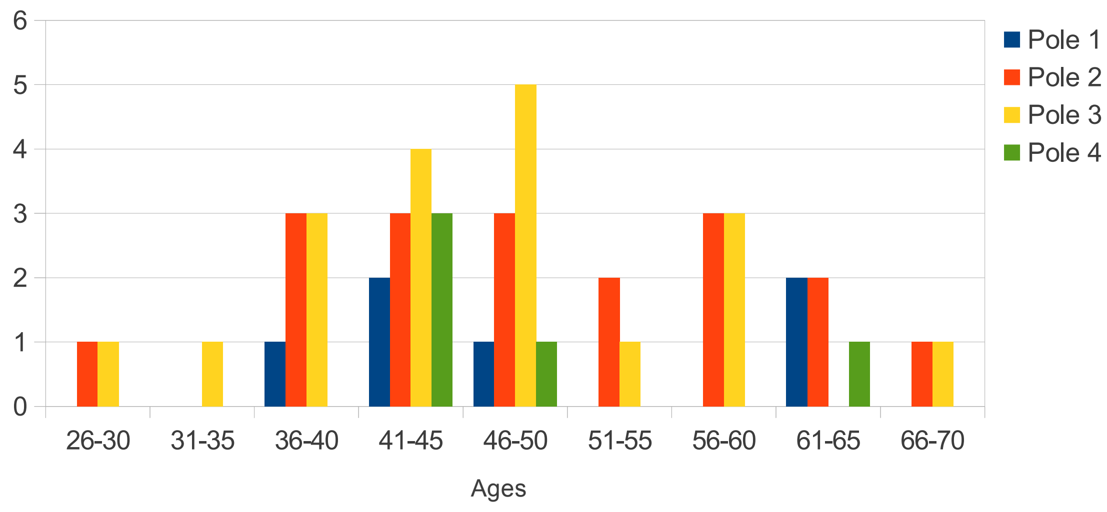


*Fig. 2.2: Age distribution per Thematic Pole of the research and teaching permanent staff currently committed to the LERMA² project, as of January 1st, 2014.*

## 2. Resources needed for the project implementation

| Pole | Scientific Themes | Needs |
|---|---|---|
| **1** | Early Universe : re-ionisation | CNRS 17 or CNU 34 (UPMC): simulation and modelling |
| **1** | Galaxy formation: early galaxies and secular evolution | CNRS 17 or CNAP SO2: ALMA observations and modelling |
| **1** | AGN and Galaxies : Feeding and Feedback | CNRS 17 or CNU 34 (UPMC): simulations and multi-λ observations |
| **2** | Laboratory astrophysics and plasma physics. Experiments | CNRS 4 or 17 or CNU 30/34 (UPMC): Priority at UPMC with Plas@par LABEX. |
| **2** | MHD simulations of the physics of star and planet formation and stellar interiors | CNRS 17 : One of the priorities of Observatoire de Paris and ENS-ICFP. Exploitation of MesoPSL. |
| **2** | Models of interstellar processes and environments (e.g. PDR, TDR, shocks, ..) for the interpretation of data from large facilities (Herschel, ALMA, GAIA, NOEMA) | CNRS 17 or CNAP : SO5 (Development of VO Theory ISM-JETS platform). Unique modelling expertise of LERMA |
| **2** | Scientific preparation and exploitation of the next generation of instruments (e.g. ALMA, NOEMA, SKA, CIDRE) | CNRS 17 or CNAP SO2 / SO3. To maintain leadership and expertise in observational sub(mm)/radio astronomy |
| **2** | Non linear astrophysical Dynamics | Professor ENS (Replacement of S. Balbus) |
| **2** | Astrophysics and plasma physics | PR 30/34 (UMPC) Development of Plasma physics at UPMC |
| **3** | Heterogeneous chemistry | CNU 30-34 (UCP) experimental research |
| **3** | Gas-grain interactions: Surface physics and photochemistry | CNRS 04, 13: Laboratory molecular Astrophysics LabEx MIChem |
| **3** | Molecular parameters for planetary, terrestrial atmospheres and ISM | CNRS 04 or CNU 30 (UPMC): New technique and developments for high resolution molecular spectroscopy. |
| **3** | Molecular Physics | PR 30 (UMPC) |
| **3** | Theoretical Molecular Dynamics | CNAP SO5 : Complex systems for astrophysical application. Support to « Service Diffusion de Données Moléculaires » and VAMDC. |
| **4** | Cloudy Earth Atmosphere | CNRS 19 : Preparation of ICI mission. Microwave remote sensing (ice clouds) |
| **4** | THz Instrumentation research | CNRS 8 or CNAP SO2 or CNU 63 (UPMC) |

| Pole | Scientific Themes | Needs |
|---|---|---|
| 4 | SIC Continent surfaces | CNRS 19: large scale hydrology via remote sensing |

## 2.3. Technical positions

The LERMA² constituting entities have developed cutting edge expertise in instrumentation, laboratory experiments and in computing science technologies. Because of new restrictions of maximal contract duration, retirements or transfers, the risk of losing some of key expertise is high. It is vital for the laboratory that the strategically most critical ones be consolidated.

In addition keeping an efficient administrative team is also critical, given the arrival of new teams and the fact that the number of research contracts keeps increasing.

| Years | Scientific Themes & Services | Needs |
|---|---|---|
| 2013 | Pole 3 : FORMOLISM - technical manager of the experimental platform | IR BAP C – Senior Supervisor |
| 2013 | Pole 4 : Remote sensing: signal processing and data inversion expert | IR BAP E – Expert in scientific computing |
| | | |
| 2014 | All Poles : Virtual Observatory (Theory) architect | IR BAP E – Expert in scientific computing (transfer from LUTh) |
| 2014 | GEMO (Pole 4) : Lead of Major Instrumentation (CIDRE, SWI, ISMAR) | IR BAP C – Instrumentation design and manufacturing (retirement of G. Beaudin) |
| 2014 | All Poles : Numerical Physics, Algorithms, New architectures | IR BAP E – HPC engineer (retirement of 2 UPMC technicians) |
| 2015 | Poles 2&3 : Technical assistance to laboratory physics and astrophysics experiments (UPMC) | AI BAP C – Experimental physics |
| 2015 | Support Pole : Administration | T BAP J - Financial Assistant (retirement of MF Ducos) |
| 2016 | Support Pole : System Administration | IE BAP E (retirement of D. Zidani) |
| 2016 | Consortium VAMDC : Project manager/chief software expert | IR BAP E - Expert in scientific computing |
| 2017 | Poles 1&2 : Data modelling and signal processing | IR BAP E – Expert in scientific computing (retirement of M. Caillat) |

## 2.4. Office Space

### 2.4.1. Paris Observatory

The LERMA² current office space at the Port-Royal campus of the *Observatore de Paris* is too limited to correctly host our PhDs and post-docs, making it impossible to host short term undergraduate students. It also does not offer international standards to our visitors. In addition LERMA² strongly wishes to diminish the number of sites where possible, in order to improve scientific synergies, internal communication and to simplify administration. Therefore LERMA² needs to have additional office space on the Paris campus of the Observatoire, our principal hosting institution, in order to improve the current working conditions of the staff presently working there, and to enable the move of the staff currently working in Meudon, in good conditions. For an estimate of 9 scientists on permanent positions, 8 non-permanent staff members (PhD, Post-Doc and engineers), plus temporary visitors and interns, as well as a small amount of shared space, the minimal office space needed is 300 m²).

In addition the experimental platforms dedicated to heterodyne measurements are currently saturated by the R&D programs. Further instrumental programs will require minimum integration facilities, which cannot be implemented on the current available surfaces. Therefore, some additional square meters should be made available to LERMA² in the Lallemand building.

### 2.4.2. ENS

With the planned renovation of the ENS laboratory buildings rue Lhomond, the distribution of office space at the ENS Physics Department will be modified. It is necessary to be attentive to the re-allocation of office space after renovation, so that LERMA² keeps a strong presence at the ENS Physics Department, both for the teaching and research activities.

### 2.4.3. UPMC

UPMC premises are in good match with the needs of the current teams (LPMAA) and of the LERMA team (plasmas and astrophysics activities). The sole issue is the need to plan specific funding for the equipment of the new offices and laboratories. The UPMC Ivry site of LERMA will be closed as soon as the new premises are available.

### 2.4.4. UCP

UCP premises need some serious renovation work related to air-conditioning, heating and office space conditions. These issues will be adressed in the next quinquennal.

## 2.5. Promotion of Research Results outside of the Academic Field

- Industrial links will be maintained and even increased through our doctoral training plans (in collaboration with Astrium, Thales, the French SME's Artenum and ABmm, the German company RPG GmbH, et c.

- A starrt-up company (Estellus) was created from the joint work carried out in the Remote-sensing group of LERMA in collaboration with LMD, *Laboratoire de Métérologie Dynamique*, and is hosted by Paris Observatory. A transfer of know-how has been signed between CNRS and Estellus. For several ESA partners LERMA and Estellus are already partners, and these links will be pursued.