CINECA

HPC Report

Cineca HPC Report 2015
website: www.hpc.cineca.it
mail: info-hpc@cineca.it

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Editorial Office
Cineca Consorzio Interuniversitario
Via Magnanelli 6/3
40033 - Casalecchio di Reno (BO) - Italy

Editorial Board
Francesca Delli Ponti
Francesca Garofalo

Design and Layout project
Francesca Delli Ponti

Print
Monograf s.r.l.
Via Collamarini 5
40138 – Bologna - Italy

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Cineca HPC Report

2015

Dear Colleagues,

for the third year I am very pleased to present the Cineca HPC Report, with the aim of continuing our commitment to offer information and data about our effort in High Performance Computing and impact on the scientific community and to share with you, and all our stakeholders, our vision and perspectives of development.

In this report for 2015, we provide an overall panorama of our activities and of the research outcomes obtained thanks to our supercomputing infrastructure both at a national and at a European level.

2015 has been a year of transition for us. New ideas were added on top of our basic goals, which were to consolidate the existing infrastructure as well as the structure of collaborations, and moreover to create the basis, by means of a public tender, to install in the course of 2016 a new world-class computing system to keep us among the top players of the HPC panorama.
New ideas and perspectives of cooperation have been targeted to put us in a even more central position in the national research system, and to see us acting like a real enabling hub, bringing value to research institutions and academia, and to the Italian industrial system.

The installation of our new Tier 0, Marconi will open the door for us to a new challenging year, for which our objective is to make our large infrastructure accessible, usable and valuable for the whole scientific community and to support national and European competitiveness worldwide.

All these targets will be achieved, clearly, thanks to our talented staff and to the strong effective and challenging cooperation with our outstanding researchers and scientists, as well as, of course, the strong support ensured by our funding agencies, to whom we will continue demonstrating the value of keeping Italian HPC at the highest level.

With kindest regards,

Sanzio Bassini
Director of SuperComputing Applications and Innovation Department of Cineca

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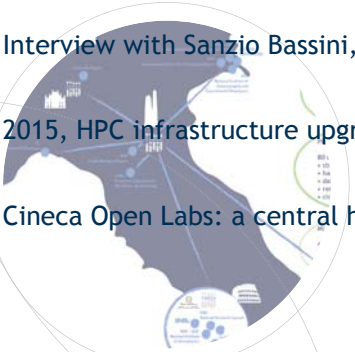

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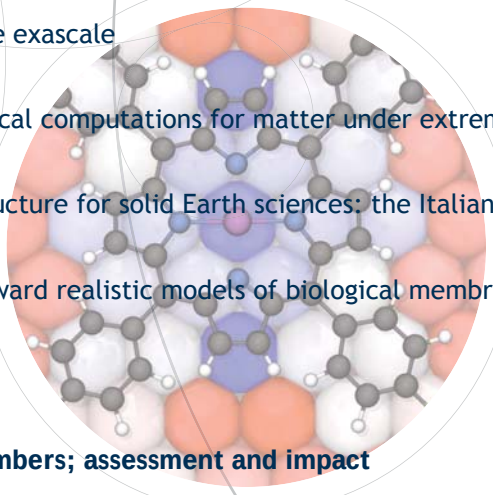

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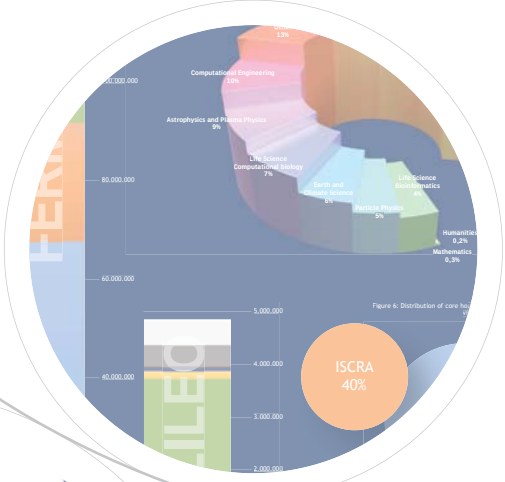

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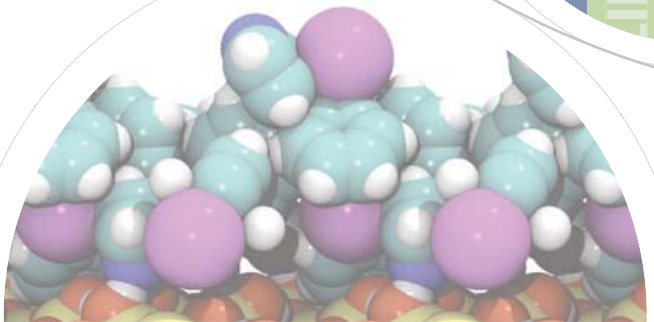


Section 1:
2015 at Cineca

Interview with Sanzio Bassini, Director of the SCAI Department of Cineca

Sanzio Bassini, Director of the SuperComputing Applications and Innovation Department of Cineca, how would you sum up in a nutshell the year 2015 for your team?

2015 can be described as a year of transition between the previous three years, characterized by the installation in 2012 of the computing system "Fermi", which for the first time positioned Italy among the “bigs” in the Top500 of HPC, and the next cycle, which has been announced already in 2016 as the year of the replacement of that system. The hope is to reaffirm an important role for Cineca and for Italy in the global HPC context for the support of research and technological innovation. During 2015 Cineca outlined an investment plan of over 50 million Euro to be valued in two technological phases over the next five years and we carried out the public tender for the acquisition of the next computing system: the logical name will be “Marconi” and the entry in production is planned for the second half of 2016. Years of transitions such as 2015, as often happens, are complex years, also for elements coming from the overall context, such as the economic crisis and difficulties of development that all Western countries have had to face and overcome.

Do you think the crisis that in recent years has hit Europe, and the Western countries in general, has had an impact on the world of HPC and its technological development?

For sure we have all observed a reduction of investment both in the upgrade of the systems of large supercomputing centers, and in terms of technological innovation. As for the large supercomputing centers worldwide the decreased investment becomes evident from the growth trends of the Top500 that, for the first time since its establishment, presents in November 2015 a certain decline. On the other hand investments in HPC technology innovation also decreased. Consequently we have seen some delay in the release of the technological components, microprocessors, systems of interconnection and data movement. The innovation of these components is essential to overcome the technological obstacles in the energy efficiency improvement of supercomputing systems, the biggest challenge on the path to exascale-class systems.

This situation has also influenced the choices of Cineca?

Of course! The facts mentioned above are one of the causes of the shift forward in the replacement of Fermi. The general availability of new microprocessors and new floating point accelerators, which exhibit very interesting data of performance per Watt of power consumption, is indispensable for the sustainability of not only the investment required for the acquisition of the computing system, but also, later of the costs for running the system.

And the impact on the world of research?

The system of public and private research consists of all our stakeholders. The hard times, which we hope are now behind us, have opened new fronts of global socio-economic challenges. Examples are the challenges of renewable energy, management and mitigation of the impact caused by the effects of climate change, or personalized medicine in order to reduce the overall costs of health systems and the broader challenge of the innovation of the materials. These challenges require enormous computing resources and represent a significant opportunity of development for the near future, after a decline in investment in scientific research as well. The research eco-system has reacted on one hand by urging the large supercomputing centers like Cineca for a process of greater focus, on the other hand to take advantage of the processes of transformation in place, such as the increasing demand for cloud computing solutions, for meeting the needs of digital infrastructures for computing and management of big data, now of strategic importance, as scientific research becomes increasingly data-driven. In any case, the economic resources have undergone a certain decline both nationally and at the European level, as evidenced by the significant reduction of the budget available for the Framework Programme Horizon 2020 in comparison with the previous 7th Framework Programme.

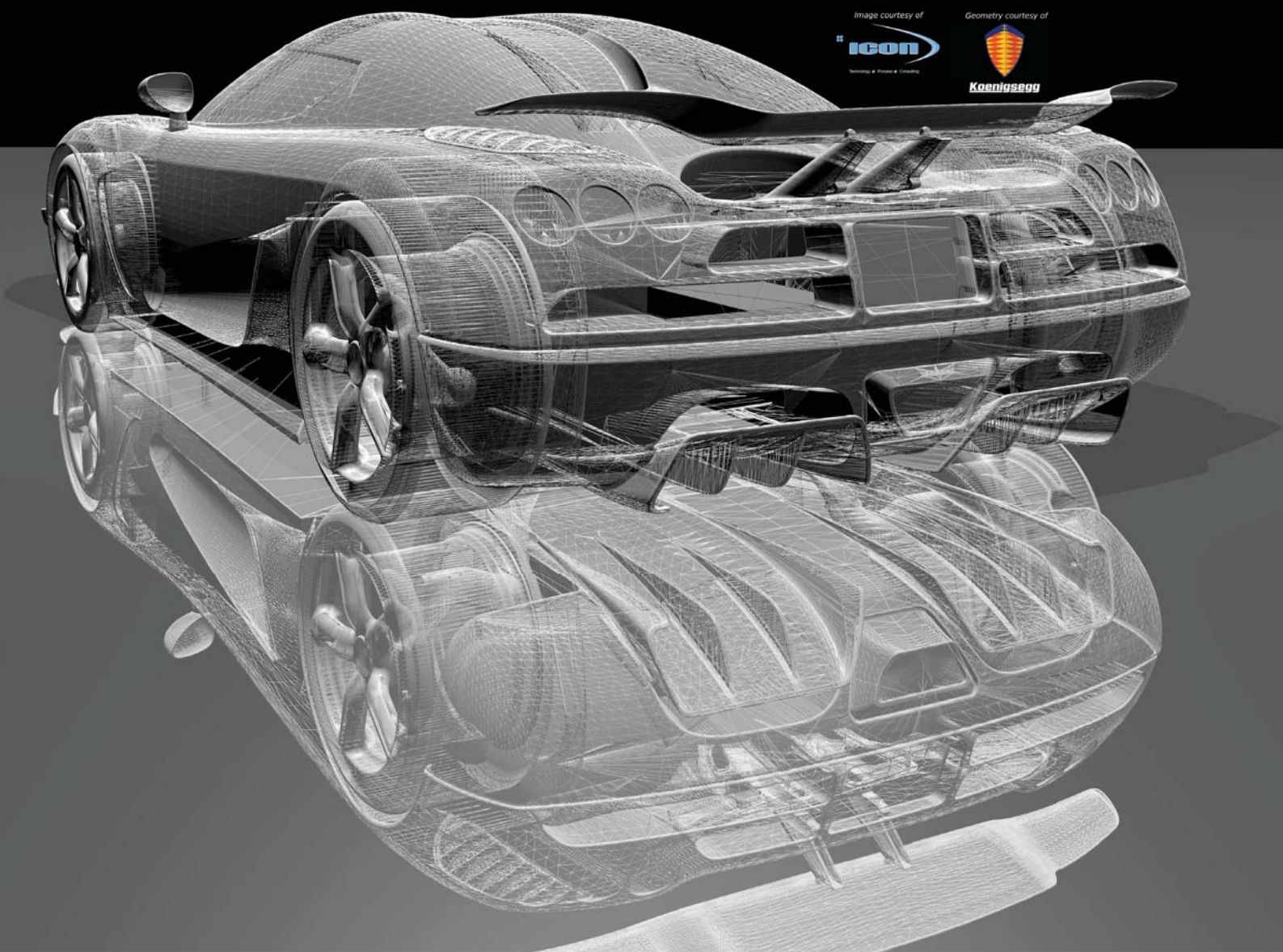
So the global difficulties may have had an impact also on the Pan-European joint research initiatives?

There is no doubt that the lower mobilization of financial resources for the digital research infrastructures for computing and data, both those made available by the member states and those from the European Union has impacted heavily on our field of action. Thus, we have seen an increase in competition for obtaining funding (e.g. actions like HPC-Europa for the trans-national access to HPC suffered an interruption in funding at the beginning of H2020, which we hope to recover in the second call in early 2016), at the same time making the process of consolidation of infrastructures and their persistence more difficult. An example is the process of finalizing the agreement for PRACE 2, a strategic and essential infrastructure in the European scenario of HPC, delayed by the lack of new funds at the European Commission level and by the need to find a way for a clear commitment by member states to transfer funds towards the PRACE AISBL. This with the aim of a fair yearly burden-sharing on all member states and not only on the hosting member countries. In fact, the agreement for the second period of operation of PRACE, for reasons of allocation of economic resources, especially by some of the smaller countries more stressed by the crisis, has not proceeded at the pace expected. Despite this, we are now coming to the final agreement, scheduled for the first half of 2016.

In your SCAI Department, how did you react to the crisis?

First of all by invoking the statutory identity of Cineca and the institutional role of the Department. In years of transition, disharmonious actions, undertaken in an attempt to overcome the difficulties that arise, can facilitate positioning errors, and Cineca has not been immune from such influences. Reorganization movements in the structure of Cineca had such an impact also on the SCAI Department, and have not always produced the expected results. The constant recall to the institutional identity represented in each case is an important driving force, which has allowed us to consolidate the activities of SCAI and to lay the groundwork for a speedy recovery of which we can already see some signs. Despite the difficulties of this year, we signed a number of cooperation agreements, for example with the Telethon foundation for rare deseases, ISTAT, National Institute of Statistics, and Unipol, the insurance company, in the field of big data, with INFN, INGV and INAF, in the field of digital infrastructures for research and with the CNR in the center of excellence for materials. We also renewed a framework agreement with the Lombardy Region.

Courtesy of Koenigsegg
HPC-Cloud-based simulation of sports-car aerodynamics
The challenge facing Koenigsegg was to perform simulations of the flow over its hypercars which were sufficiently detailed to model real physical effects accurately.



We used to say that from crisis opportunities may arise. What opportunities and plans are foreseen for 2016 and beyond?

I mentioned a number of joint development agreements. Besides these, that are expected to produce significant results over the next year, 2016 will be characterized by a strong focus on infrastructure. The investment plan designed by Cineca will be extended over the next year for the start of the HPC service for Eurofusion. That's a brilliant result that the Department took over in 2015, winning the international public tender for the HPC service to the worldwide community of Eurofusion, provided by Cineca for the next four years thanks to a project presented with Enea.
It will also be the year to lay the foundations for a fruitful renewal of the framework agreement with Eni and will be the year in which the foundations are laid for a gear change at national level for the persistence of the digital infrastructures for research. We said "crisis as an opportunity". Certainly the crisis has affected all of us and also entities such as GARR and INFN may have been affected. It might, in this case, be agreed that there is the need to better define each one's role and in that sense, the logic of avoiding competition with each other: I think that we would create great value by integrating the infrastructure of GARR, for the network and data transport, of CNAF - INFN, for the services of High Performance Throughput and LHC data, and Cineca for the HPC and data of the national research system as a whole. This would build a structure that is a quantum leap for a concrete contribution towards the "Digital Single Market" open to all researchers and all disciplines.

To conclude this interview, what are your opinions and ideas of development for the future?

HPC has transformed the way we do research and innovation, and on the other hand research, its needs and its project capacity, all rely heavily on HPC. First, even if we are not changed by the crisis, we should at least become more responsive. To be effective we need a continuous assessment on KPI inside and outside Cineca, referred both to the performance and production of computing systems, and to the excellence performance of all the resources and expertise available in the Department and in the HPC ecosystem around Cineca. So it will be essential to have a very powerful assessment ability to be able to highlight the impact of HPC with politicians, executives, opinion leaders and potential funders (the tax-payers). Secondly, we must move towards a greater flexibility in interpreting the management of the supercomputer systems. The concept of the Digital Single Market will become reality anyway and those who are out will suffer a recurrence of crisis situations. The convergence of big data and supercomputing is already proposing a wide range of ways to access the systems of large scale facilities where HPC and Data Analytics converge, giving greater weight to the promise for methods of machine learning and cognitive computing. These methodologies will be certainly a recurring leitmotif in the HPC transformation and widening process. Finally, as regards the gradual emergence of new scientific methodologies for the traditional HPC, this will produce an effect on the service model: the open access subject to peer-review will be consolidated, but with more attention to communities and scientific challenges rather than the individual projects. Moreover a model of "google-like" access, open and free, will be increasingly present and will fundamentally alter HPC, giving increasing importance to the overall productivity.


Procurement of next Tier-0 in progress
FERMI - IBM BG/Q
10K computing nodes
160K cores
2 PFlop/s Peak Performance
PRACE Tier 0
GALILEO - IBM/Lenovo NeXtScale Cluster
512 nodes, Intel Haswell
8K cores
768 accelerators (Intel
National Tier 1
PICO - IBM NeXtScale Cluster
80 computing nodes
• structured and unstructured data processing
• hadoop and map reduce
• data insight
• remote visualization
• cloud computing
High Performance Data Analytics
MULTI TIER STORAGE
40 TB fast (SSD) storage
5 PB GSS storage
12 PB TAPE storage, integrated with GSS through LTFS
Data repository, curation and preservation
SISSA - ISAS
International School for Advanced Studies
ELETTRA SINCROTRONE
ICTP
International Centre for Theoretical Physics
Lombardia Region
OGS
National Institute of Oceanography and Experimental Geophysics
CINECA
IIT
The Italian Institute of Technology
RER
Emilia Romagna Region
LENS
European Laboratory for Non-linear Spectroscopy
CINECA
CNR
National Research Council
ENEA
INAF - IASF
National Institute of Astrophysics
Civil Protection
INFN
National Institute of Nuclear Physics
CMCC
Euro-Mediterranean Center on Climate Change

2015, HPC infrastructure upgrade

2015 has seen a consolidation of Cineca High Performance Computing infrastructure.

The IBM-PLX system has been replaced by Galileo, an IBM NeXtScale cluster equipped with Intel Haswell processors and Xeon Phi accelerators. The system, classified as Tier 1 within the European PRACE Research Infrastructure, is aimed at hosting both technical and academic workflows. The production on the cluster is quite heterogeneous, ranging from CFD applications, to weather forecast simulations, from ISCRA scientific projects to risk and finance simulations. Capable of a theoretical peak performance of 1,100 TFlop/s and 684 TFlop/s sustained peak, Galileo has reached the 130th position in the Top500 list of most powerful computing systems in the world as in November 2015. From the user perspective, Galileo offers a unique feature: it is the first Cineca system to provide researchers with nodes that host Intel Xeon Phi accelerators for testing and production. The Xeon Phi belongs to the many integrated cores (MIC) architecture which combines many Intel CPU cores onto a single chip. A MIC card can be seen as a coprocessor, meaning that processor units can offload to MICs most - or all - the intensive computing part of a simulation. Each MIC card supplied with Galileo features 60 physical Intel cores at 1.2 GHz and 16GB of memory. These cards, codenamed Knights Corner - KNC - constitute the second generation of the Intel MIC roadmap, that will see a further evolution with the release of Knights Landing - KNL - in 2016. KNL is expected to improve KNC computational power by a factor of three: from 1 to 3 TFlop/s of theoretical peak for each card. Despite the increase in performance, the thermal design power - which is an index of the heat dissipated by the card - is expected to decrease from KNC to KNL, therefore improving the power efficiency of the card. In this regard, Galileo can be seen as a prototype of one of the next generation architectural solutions that aim to close the gap between nowadays clusters and the future exascale systems.
Fermi, the IBM Blue Gene/Q system deployed in 2012, has reached its third year of production. This system has represented a turning point for the national research in computational science, being the first Italian system to enter the top 10 of the most powerful computers in the world. Fermi has boosted the competitiveness of computational researchers, providing hundreds of millions of core-hours through european (PRACE) and italian (ISCRA) grants. Fermi has almost completed its life-cycle and will be phased-out in 2016, to be replaced by a new Tier 0 system: Marconi. This is part of a two-stage, 5-year program that plans to provide a 50 PFlop/s system by the year 2019. First with a replacement of Fermi, followed by a system evolution towards the goal of 50 PFlop/s of peak performance. The procurement of the new Tier 0 system will be completed by the end of 2015, and Marconi will be ready for deployment in 2016. Cineca will also host the system dedicated to the Fusion research in Europe: a combined system providing a performance of 1 PFlop/s standard CPUs and 1 PFlop/s accelerated by the end of 2016, to be upgraded to 5 PFlop/s standard CPUs and 1 PFlop/s accelerated in 2017.

Fermi - IBM BG/Q

The HPC services provided by our infrastructure have also seen improvements in 2015. With the introduction of Pico in 2014, an increasing effort has been made to integrate all the clusters that constitute the Cineca HPC ecosystem. Galileo makes no exception in this regard. As an example, the system is fully interconnected with Pico's high capacity storage; data retained on Pico storage can be pre- or post-processed directly on Galileo, avoiding time-consuming large data movements. This is a first step towards a more data-centric High Performance Computing approach which, in our opinion, will be of great benefit for the overall user experience on our systems. The data-centric model is a recent trend in HPC based on the consideration that data produced by modern simulations will keep growing in size, raising the need of integrated solutions that allow users to produce, inspect and process data without transfer them across the HPC infrastructure or - in worst case scenario - from HPC to local systems. In this context, an effort has been made by our staff to build vertical solutions that avoid data movements within a typical user workflow. For example, data produced on any Cineca HPC system can be visually inspected through the improved remote visualization service provided by Galileo that can exploit up to 160 GPUs Tesla K40.

A new High Performance Computing cloud service is available on Pico for all the users. In recent years, demand for scalable compute capacity is growing across all areas of research. The applications and the skills to maintain them vary considerably between science teams. HPC centers that "can adapt" their infrastructures to application requirements simplify this deployment scenarios. Traditional HPC systems have limited capabilities for adapting cluster environments to application requirements. To accomplish this extreme flexibility of its computing services, Cineca introduced PicoCloud, a High Performance Cloud Computing infrastructure, based on OpenStack, that can be easily configured to support various Operating Systems and development environments, to deploy in an optimal way different kind of workloads. This architecture provides full user access to cloud instances, so users can easily tune instances to mirror application requirements and can replicate app-specific instances giving them an easy path to scale workflows on larger data sets. PicoCloud currently hosts about 25 projects, including the services of the National Research Council (CNR) for the EU project Copernicus.

Mirko Cestari and Giuseppe Fiameni
Cineca

Galileo - IBM/Lenovo NeXtScale Cluster

Cineca Open Labs: a central hub for research and innovation

It is understood that the knowledge society towards which we are aiming and evolving, in many areas, together with higher education and higher skills, requires the use of state-of-the-art technologies, and the pervasive use of computational capability as a lever to multiply the development of knowledge, especially when the knowledge society is overlapping with the information society. On the other hand, the technologies related to the computational infrastructures require an increasing investment in knowledge based innovation to overcome the physical limitations that are inevitably associated with each technology. This knowledge has long been grown within the scope of High Performance Computing. The new scientific challenges on one hand (Human Brain Project, new materials, climate change, personalized medicine...) and new technological challenges on the other (energy efficiency, miniaturization, network speed, data storage, etc...) require more and more a deeper integration and dissemination of knowledge: those problems cannot be solved staying within the perimeter of a single domain and in this respect HPC based knowledge can be a formidable instrument to accelerate the dissemination between domains.

To facilitate this dissemination and to help the adoption of HPC based knowledge by a broader audience, Cineca, for a few years has been promoting open laboratories, where this is made possible and where technologists, researchers and application developers together, co-design solutions, applications and the best ways to exploit them.

In the Open Labs experts from a given domain work together with experts in HPC technologies, and they co-design HPC solutions for that domain. The outcome of the Lab is a stronger application or technological solution that brings benefits to a broader audience, not only limited to the specific domain. The Open Lab is in fact open to receive input and to promote technology transfer solutions towards third parties including industries and especially SME, usually not having the resources to exploit HPC technologies on their own. Then, in the Open Lab there is tipically the coexistence of three main stakeholders, the structured research from academia or national research institutions, having the scientific leadership of the Lab, the HPC experts form Cineca, contributing in the implementation of the application and/or solution, plus a third party (public or private) representing the user of the solution. This picture is sometimes an oversimplification of the real status of the Open Lab, where the boundaries between these roles are not always so sharp.

In respect of the Open Labs, Cineca plays the role of a research and technology transfer hub where solutions developed in one of the Labs can be exploited in another Lab maximizing the impact of the HPC infrastructure and of the knowledge of the people on the scientific, societal or industrial challenge.

The process of implementing the Open Labs structure is ongoing, with some Labs already working and some other under definition. In total Cineca is planning to support the start-ups of 4/5 Open Labs in the following domain: energy efficiency, material science, fundamental physics, geoscience, big data analytics, genomics/life science.

In particular three Open Labs have already been implemented, energy efficiency, material science, big data analytics, having an immediate impact on the respective domain and winning by important EU funds.

The Lab on energy efficiency in HPC has been established together with the team of prof Luca Benini of University of Bologna and ETH Zurich. The goal of the Lab is to study solutions for maximizing the energy efficiency of current and future HPC technologies. The outcome of this activity is particularly relevant for the future and sustainability of HPC itself since, today, the main constraint for the implementation of more powerful supercomputers is the energy required to power them. Besides the HPC, the knowledge and the solutions developed by the Lab have important impact in other domains as well, from a better design of datacenters to the best design for personal devices, internet of things, strategies scheduling and big data. In fact, the first step to have a good energy efficiency strategy is to implement a fine grain energy consumption monitoring infrastructure. But since the number of components to be monitored in supercomputers is in the order of several millions, internet of things strategies for collecting the results and big data tools to analyze them are required. Moreover this Lab was able to setup EU projects that has been funded by the H2020 programme (ANTAREX), with the goal to develop innovation into compilers to develop auto-tuning applications.


CINECA
hub for innovation and research
HPC energy efficiency
technology transfer
big data analytics and management
condensed matter and solid state physics
fundamental physics
environmental science
bioinformatics and life science
stakeholders
EU funded research
MONT BLANC
DEEP
Intel® PCC
ANTAREX
ETP 4 HPC
OpenPOWER
eni
Dompé
FORTISSIMO
PRACE
SHAPE
EUDAT
Istat
Istituto Nazionale di Statistica
Unipol
GRUPPO
MAX
QUANTUMESPRESSO
EUROfusion
INFN
Istituto Nazionale di Fisica Nucleare
EPOS
ENVRI
EMODnet
myOcean
NextData
elixir
ITALY
EPIGEN
telethon
ENEA
SISSA
Consiglio Nazionale delle Ricerche
cmcc
Consortium GARR
INGV
OGS
ICTP
International Centre for Theoretical Physics
exdci
EuHIT

Material Science

Materials are crucial to scientific and technological advances, industrial competitiveness, and to tackle key societal challenges - from energy and environment, to health care, information and communications, manufacturing, safety and transportation. Moreover the accuracy and predictive power of materials' simulations based on "first-principles calculations" allow nowadays a paradigm shift for computational design and discovery, in which massive HPC and HTC (High Throughput Computing) efforts can be launched to identify novel materials or materials with improved or designed properties and performances.

Given that Cineca has established an Open Lab for the research of innovative materials with the aid of high-end HPC technologies, the Lab is collaborating with the MaX European center of excellence led by CNR with prof Elisa Molinari as PI. This is the only EU centre of excellence led by an Italian institution. This Lab is also supported by the collaboration between Cineca and Intel for software modernization to prepare the applications used in material science for future generations of supercomputers. In particular within the activities of the Open Lab there are two community codes where Cineca is investing effort, Quantum Espresso and Yambo, representing also a large fraction of the production on Cineca HPC systems and other EU centers as well.

Big Data

Scientific real and computational experiments, sensors, devices, and digital social behaviour of people are all producing a growing amount of data that, if properly managed and analysed, could produce new knowledge from the data. Key critical factors are the capability to store and preserve large volumes of data and the computational capacity to speed-up the analysis of the data themselves. These are not the only relevant factors but are those that can be addressed by "traditional" HPC infrastructures. The collaboration with scientists and researchers from public and private institutions and HPC expert to tackle together the challenges and the opportunities relative to the new methods of finding new knowledge in the data is then natural. Cineca is setting up and promoting an Open Lab on this subject in collaboration with prof Sonia Bergamaschi from the University of Modena and Reggio Emilia. The infrastructure of Cineca itself has been changed in light of the growing relevance of the data, and a dedicated system (Pico) has been implemented to support "Big Data" and "Cloud" applications. Many communities are starting to use the new system and the services implemented within the Open Lab and bring their data to the storage system integrated in Pico and use its computational performance to process them. Pico represents the largest infrastructure for this kind of applications publicly available to the Italian research community.

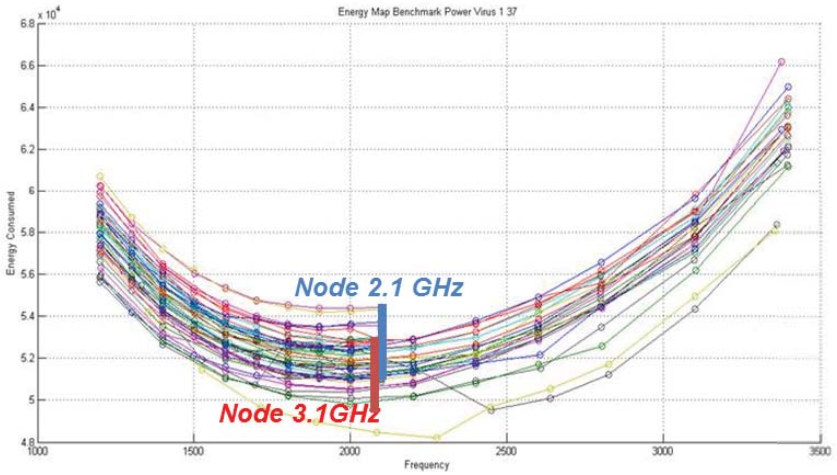
The activities of the Lab have included also a Proof of Concept in collaboration with UNIPOLSAI with the goal of speeding-up and improving the accuracy of the risk management process.

Other Labs are in a preliminary stage, but we plan in 2016 to start at least two further Labs, one for geo-science and one for bio-informatics and life science, both with the important goal of making the role of Italy stronger inside EU initiatives like EPOS and ELIXIR.

The structure of the Open Labs working with Cineca as a central hub favour technology and knowledge transfer among the Labs and collaborations occur naturally among them, since HPC related technology is by nature transversal to the domains. Indeed the three Labs already started have begun to collaborate multiplying the impact, the competitiveness and the effectiveness of the activities of the Labs.

The Open Labs have proved to be particularly effective in improving the fund rising capability with respect to the same entities and people working alone, mainly due to the fact that working in the hub the competence and the knowledge are shared and allow better projects with higher impact. For the national system as a whole this is a great opportunity to be more competitive with respect to other international players, and closing the gap with the leaders.

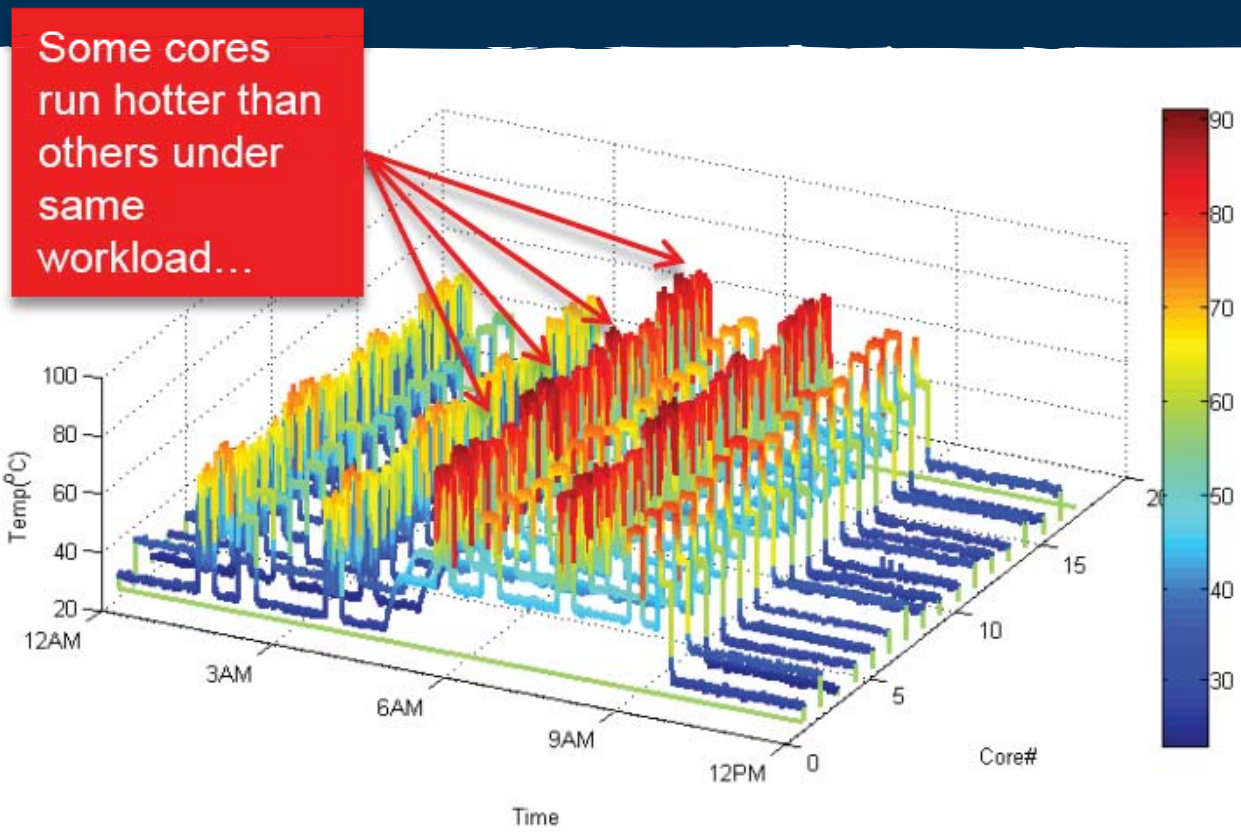
Carlo Cavazzoni
Cineca



Energy consumption (y-axes) for the same CPU bound task when running in all the eurora nodes (different line) at different clock frequency (x-axes).
We can notice that the different nodes shows a energy variability of almost the 10% and that 3.1Ghz cpus are in average more efficient than the 2.1 Ghz cpus when operating at similar frequencies. Moreover for cpu bound applications the most energy efficient operating point is not the most perfoming one. Compared to turbo frequency operating the cpus at the optimal frequency (2.0GHz for this benchmark) leads to almost the 27% of energy saving.

Energy efficiency measurements on Eurora system, for the Green500 submission. Nota that at the end Eurora was ranked in the first position being, at that time, the most energy efficient supercomputer in the world.

Eurora thermal heterogeneity. Even if liquid cooling is capable of uniformly cool all the nodes of the eurora system the different processing elemement form factor and unavoidable manufactury variability leads to different thermal resistance inside the node in between different nodes. Thermal resistance measure the heat removal efficacy for the given component.



MAX: materials design at the exascale

Materials are crucial to scientific and technological change and industrial competitiveness, as well as to tackle key societal challenges – from energy and the environment to health care, information and communications, industrial processes and manufacturing, safety and transportation. The increasingly high accuracy and predictive power of computer simulations combined with increasingly higher levels of computing power and large amounts of storage capacity of High-Performance Computing (HPC) technologies, now enables a paradigm shift in material design and discovery, in which every increasingly complex material behaviour will be addressed by easily accessible, interdisciplinary, easy-to-use computational experiments.

MaX (Materials design at the eXascale) is a user-driven European Centre of Excellence (ECoE) established to support developers and end-users in materials simulations, design and discovery. MaX focuses in enabling the best use and evolution of HPC technologies by creating an ecosystem of knowledge, capabilities, applications, data workflows, analytic tools and user-oriented services.

At the same time, MaX is enabling the exascale transition in the materials domain, by developing advanced programming models, novel algorithms, domain-specific libraries, in-memory data management, software/hardware co-design and technology-transfer actions.

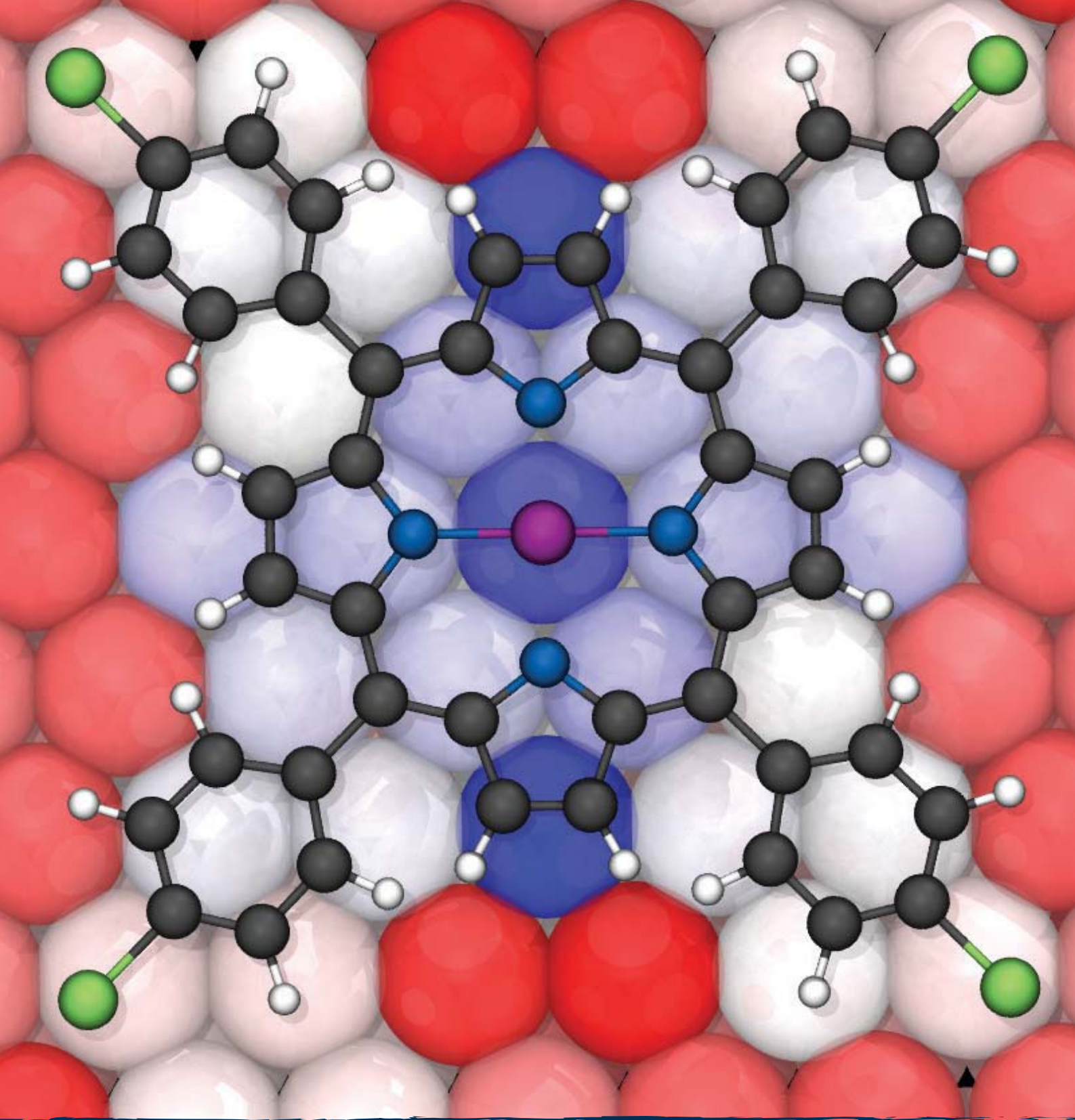
MaX is designed and managed to support the needs and the visions of a number of players:

- **End-users** in research and innovation, both in industry and academia, who explore materials discovery and rely on computer experiments.
- **Domain scientists** who develop new methods, algorithms and tools in materials simulations.
- **Software engineers** and **vendors** who optimise hardware and software performance and usability together with analytical tools for increasingly efficient computer-assisted materials design.
- **HPC centres** and **industry** who are interested in empowering the most advanced and ambitious solutions and in hardware-software co-design.

The MaX implementation strategy consists in developing a new application and data ecosystem, and serving its industrial and academic community through end-user oriented actions. MaX key actions include:

- Implementing a **Sustainable Programming Platform** designed to develop quantum engine kernels and low-level domain specific libraries, to facilitate quantum engines' advanced functionalities and to share libraries with other communities/domains.
- Building a **Dynamic Data Framework** to manage the automation of high-throughput calculations, automatic data storage, workflows interchange where data provenance, preservation, reproducibility, and reuse are guaranteed.
- Promoting the **Exascale Transition Enabling Action** through the development of novel algorithms, domain-specific libraries, in-memory data management, and software/hardware co-design.
- Establishing the **User Needs and Solutions Integrating Protocol** by aligning the technological offer with leading end-users requirements.
- Developing a **Catalogue of Services** accommodating end-users help-desk and support, communities' integration, industrial outreach, custom development and consulting.
- Contributing to the diffusion of material simulations by addressing the skills gap through an integrated offer of **Training and Education** programs in HPC and computational material science.

MaX initially focuses on selected flagship codes: widely-used applications, based on rather diverse models, mainly oriented to structural, electronic, magnetic properties and to spectroscopies of materials from first principles: *Quantum Espresso*, *Siesta*, *Fleur*, *Yambo*. A further application, *Aiida*, is the basic informatics infrastructure adopted and developed for workflow and data management, preservation and sharing. MaX will expand the potential of these flagship codes on the present HPC platforms, by implementing new capabilities and algorithms for the the study of complex materials, properties and processes in realistic condition, far beyond the current realms. At the same time, MaX will enhance the performance of the flagship codes in terms of scaling,



Spatially Extended Kondo State in Magnetic Molecules Induced by Interfacial Charge Transfer. Phys. Rev. Lett. 105 106601 (2010). Courtesy of H. Kulik

robustness, and usability, and will make them ready for the forthcoming exascale hardware architectures. In this way, MaX is designing and implementing a sustainable approach of relevance beyond its core codes and field.
MaX will act as a central service hub that will provide project management, coordination and dissemination management for each of the project members, shifting and reducing costs by sharing resources and effort. To guarantee the quality of the provided services MaX will maintain toolsets, templates, and documentation of best practices, procedures, and techniques.
A number of 'Pilot Cases' will be developed in close contact with leading industrial partners representing a challenging test ground for the MaX working approach. The developed packages and work-flows emerging from the Pilot Cases experience will constitute the basis for a 'market-place' where solutions developed for a given problem will be made available and tailored to other end-users. This opportunity is expected to enable rapid response to shorter-term issues, and could be typically well suited e.g. for SMEs.

Guido Chiarotti and Elisa Molinari

MaX Materials at the exascale - European Center of Excellence

MAX DRIVING THE EXASCALE TRANSITION

The MaX logo and payoff. MaX communication strategy is aimed at developing a unified and coherent MaX image to enhance community identity among stakeholders. MaX communication style is simple, direct, clear and geometrical. It makes extensive use of basic geometric shapes and of the *less is more* concept in communicating, teaching, and programming.

MaX partners include 5 research institutions: CNR Modena, SISSA Trieste, ICN2 Barcelona, FZ Jülich, EPFL Lausanne. 5 supercomputing centres: CINECA Bologna, ETH/CSCS Zürich/ Lugano, FZ Jülich, KTH Stockholm , BSC Barcelona. 1 global research & education institution: ICTP Trieste. 2 SME business partners in hw and open source technologies: E4 Computer Engineering Scandiano (Reggio Emilia), CloudWeavers London.

MaX is one of the eight 'European Centres of Excellence for HPC applications' supported by the EU under its H2020 e-INFRA-2015 call, GA: 676598.

QUANTUMESPRESSO
www.quantumespresso.org

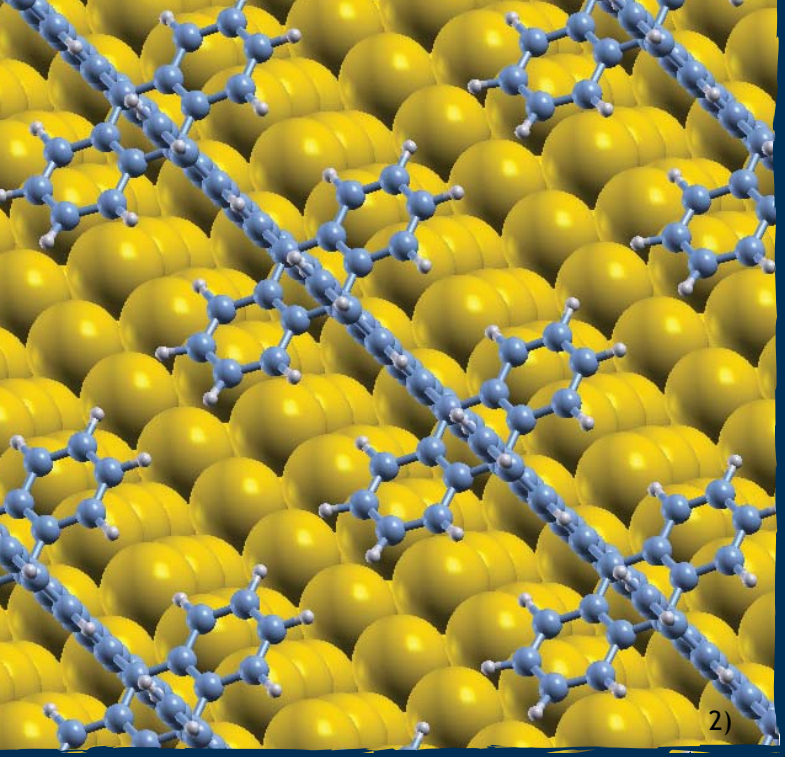
Yambo
www.yambocode.org

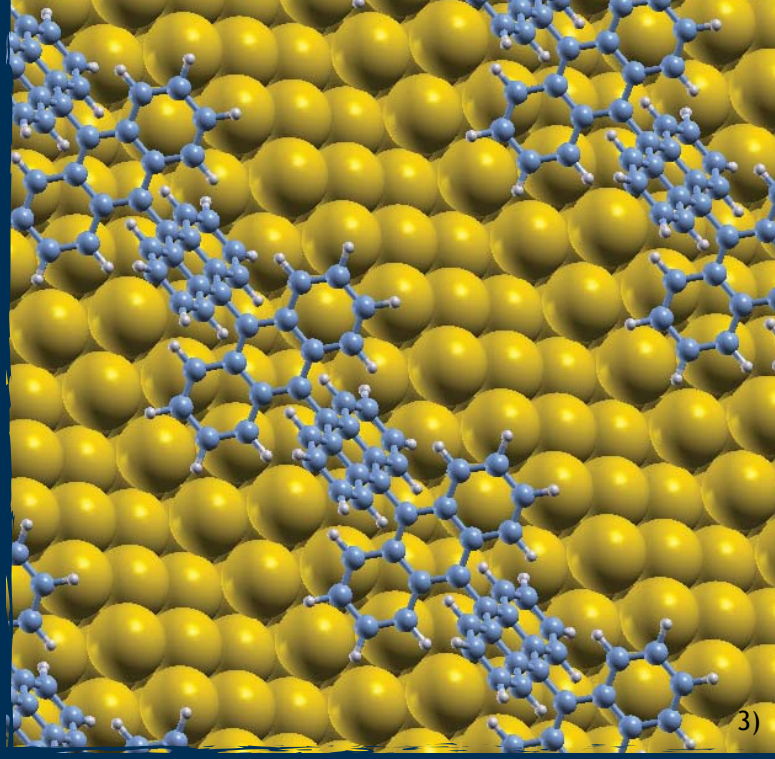
siesta
www.icmab.es/siesta

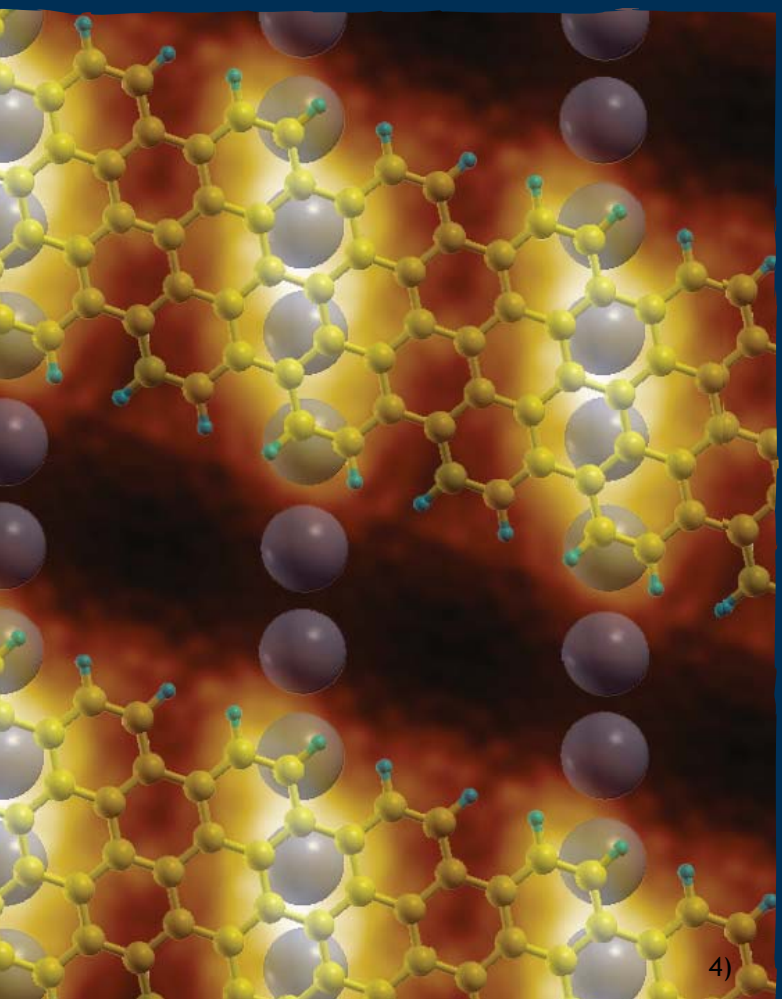
fleur
www.flapw.de

www.max-center.eu

AiiDA
www.aiida.net





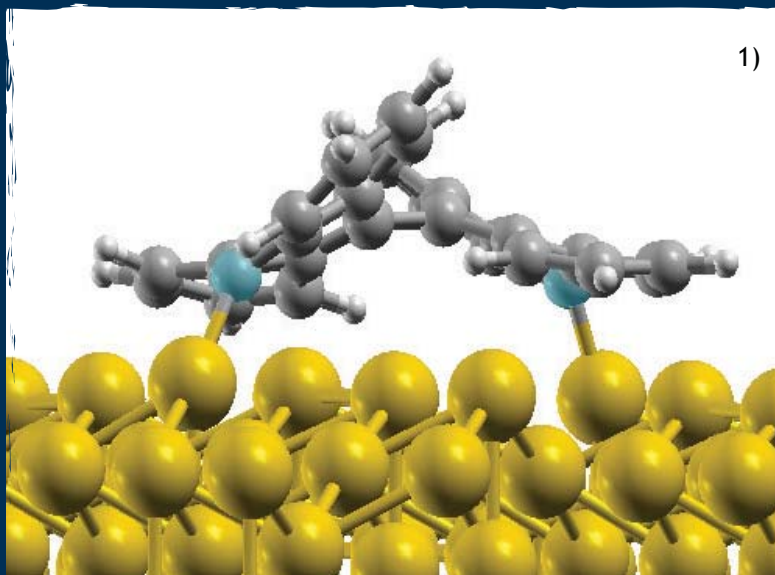


Graphene Nanoribbon Synthesis on Gold (110) Reconstructed Surfaces.
Courtesy of A. Ferretti.

1)
DBBA Precursor

2 - 3)
Polyanthryl formation

4)
Simulated STM image



From INFN:
extreme numerical computations for matter under extreme conditions

Matter inside and around us is almost completely made up of nucleons, i.e. protons and neutrons, bound together into nuclei by the strongest among the known fundamental interactions of Nature. How far is that from matter filling the Universe when the temperature was well above one trillion Kelvin degrees, or present in the inner core of neutron stars, where pressure is more than thirty orders of magnitude higher than in our atmosphere?

Precise answers to such questions would represent fundamental pieces of our knowledge from various points of view. We need them in order to understand the evolution of the Universe during its early stages, or the properties and fate of many compact astrophysical objects. However we also need them to get more insight into fundamental interactions of Nature. For those reasons, various laboratory experiments have been devised, in which massive particles, like lead or gold ions, collide at extremely high energies, thus producing fireballs with conditions similar to the ones described above.

In order to understand the behaviour of matter under such extreme conditions, one needs to uncover the properties of Quantum Chromodynamics, i.e. the theory of strong interactions between quarks and gluons, which are the elementary particles constituting nucleons. QCD has many similarities to Quantum Electrodynamics (QED): quarks carry a new type of charge, named "color", leading to interactions mediated by gluons, which are the analogous of photons but, contrary to what happens in QED, carry color charges themselves. That makes QCD a much more complex theory with respect to QED, so that in most of the conditions relevant to our discussion analytic computations are not possible, and a numerical treatment represents the only available tool to obtain reliable predictions from QCD.

One of the most striking properties of QCD is that, in ordinary matter, no free quarks and gluons exist, but they are instead permanently confined into hadrons, like protons and neutrons, which are globally neutral under color charge. This property of strong interactions is known as color confinement. The properties of strongly interacting matter are however expected to change drastically in the presence of extreme conditions, in particular when the density of hadrons becomes so large that they start overlapping in space. That may happen either when ordinary matter is exceptionally compressed or in the presence of exceptional temperatures, for which a large thermal production of hadron-antihadron pairs takes place. A simplistic description of what happens in such conditions is that quarks and gluons start propagating from one overlapping hadron to the other; the final medium which is expected to be created, in which quarks and gluons are deconfined, has been named Quark-Gluon Plasma. Reliable predictions are however needed, in order to make such picture more precise: numerical computations provide a valid approach to reach this goal.

The basic idea is to make use of Monte-Carlo simulations and compute the partition function of strongly interacting matter. This is expressed as a path-integral, that means an integral over field configurations, which represent the stochastic variables which should be sampled by the Monte-Carlo algorithm. In order to make the simulation conceivable, the system must be discretized on a space-time lattice contained in a finite box: in this way the number of integration variables, which are represented by 3 by 3 unitary matrices connecting the different points of the lattice, becomes finite. Of course, the box size must be large enough (a few femtometers at least) and the lattice spacing small enough (a tiny fraction of a femtometer) so as to keep systematic errors under control. The possibility to perform several simulations at different values of the box size and of the lattice spacing permits to perform reliable extrapolations both to the continuum and to the infinite volume limit.

The numerical challenge is far from trivial. Realistic discretizations involve at least 10^8 stochastic variables, the hardest task being the frequent inversion of a large sparse matrix (fermion matrix) connecting vectors with a comparable number of elements: that is needed to compute the propagation of quarks. Indeed, as a consequence of the very low mass of the two lightest families of quarks (up and down), as compared to the typical energy scale of QCD (a few MeV against a few hundred MeV), the lowest eigenvalue of the fermion matrix is typically quite small and that makes its condition number not favorable.

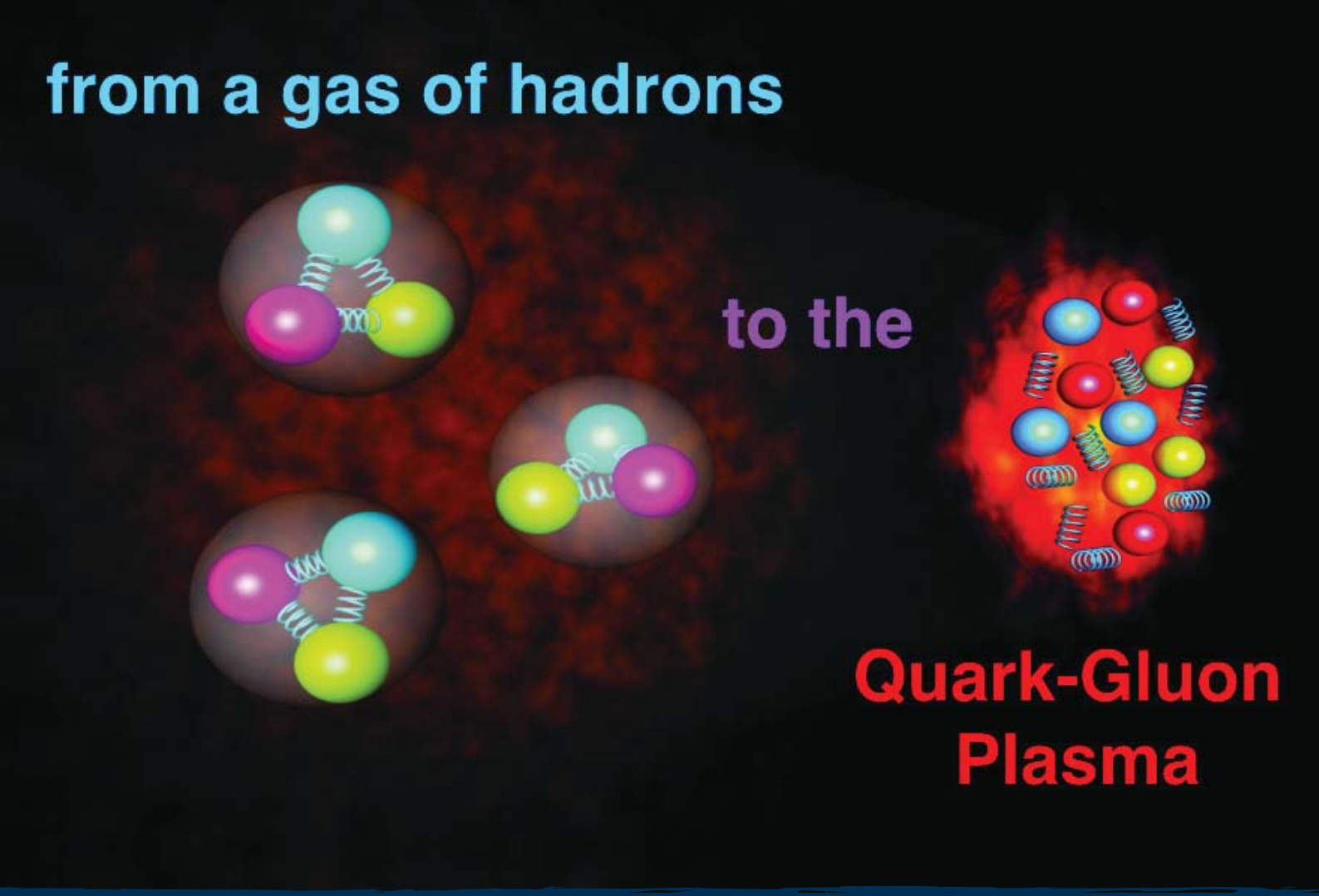


Figure 1: An artist view of the micro-world at the scale of the femtometer, showing quarks and gluons that organize as traditional hadronic matter or as a quark-gluon plasma phase, developing at sufficiently high temperature and density.

For that reason, Lattice QCD simulations represent one of the most complex problems in computational physics, indeed they have been a major stimulus to the development of High Performance Computing resources since thirty years. Nowadays, the available computational resources are powerful enough to permit realistic computations, a typical big size project requiring at least 100 Teraflops * year. This has been possible thanks to progress both on the computer and on the algorithmic side. If we look, for instance, at the development taking place in the period going from 2001 to 2012, an improvement in the peak performance of the most powerful machine by about 3 order of magnitudes has been accompanied by an even larger improvement gained on the algorithmic side (almost 4 orders of magnitude). As a consequence of such progress, we are now in a position to provide precise and reliable results for various aspects of strong interaction physics, going from the determination of hadron masses to the properties of Quark-Gluon Plasma, even if some yet unexplorable areas still remain, regarding for instance the physics at very large baryon density, due to the fact that in this case standard Monte-Carlo simulations fail because of the so-called sign problem.

In the framework of INFN research activities, lattice QCD groups investigating the properties of strongly interacting matter in the presence of extreme conditions are playing a leading role at the international level. An essential contribution to that has been represented by the ongoing collaboration between INFN and Cineca, providing access to Fermi and Galileo. Various projects, devised by INFN collaborations a few years ago only at the level of prototype simulations, have been or will be realized soon adopting state-of-the-art discretizations of strong interactions.

Some of our projects regard the properties of strongly interacting matter in the presence of strong magnetic background fields. This is relevant to many contexts, like the early stages of the Universe, a class of neutron stars known as magnetars or heavy ion collisions, where magnetic fields as large as 10^{16} Tesla might be created. In particular, we have revealed the effect of the magnetic field on the confining force between quarks [1] and that the Quark-Gluon Plasma is among the strongest paramagnetic materials in Nature [2]. Furthermore, we have provided results for the dependence of the deconfinement temperature on the baryon chemical potential [3-6], we have explored new approaches to the study of thermodynamics on the lattice [7] and we have investigated the fate of the confining forces among quarks around the pseudo-critical temperature [8]. Other exciting investigations are in progress, in order to clarify the connection between QCD thermodynamics and a candidate new particle, known as the axion, which could explain part of the dark matter observed in the Universe.

Massimo D'Elia
Physics Department, University of Pisa and INFN – Pisa

Raffaele Tripiccione
INFN and Ferrara University

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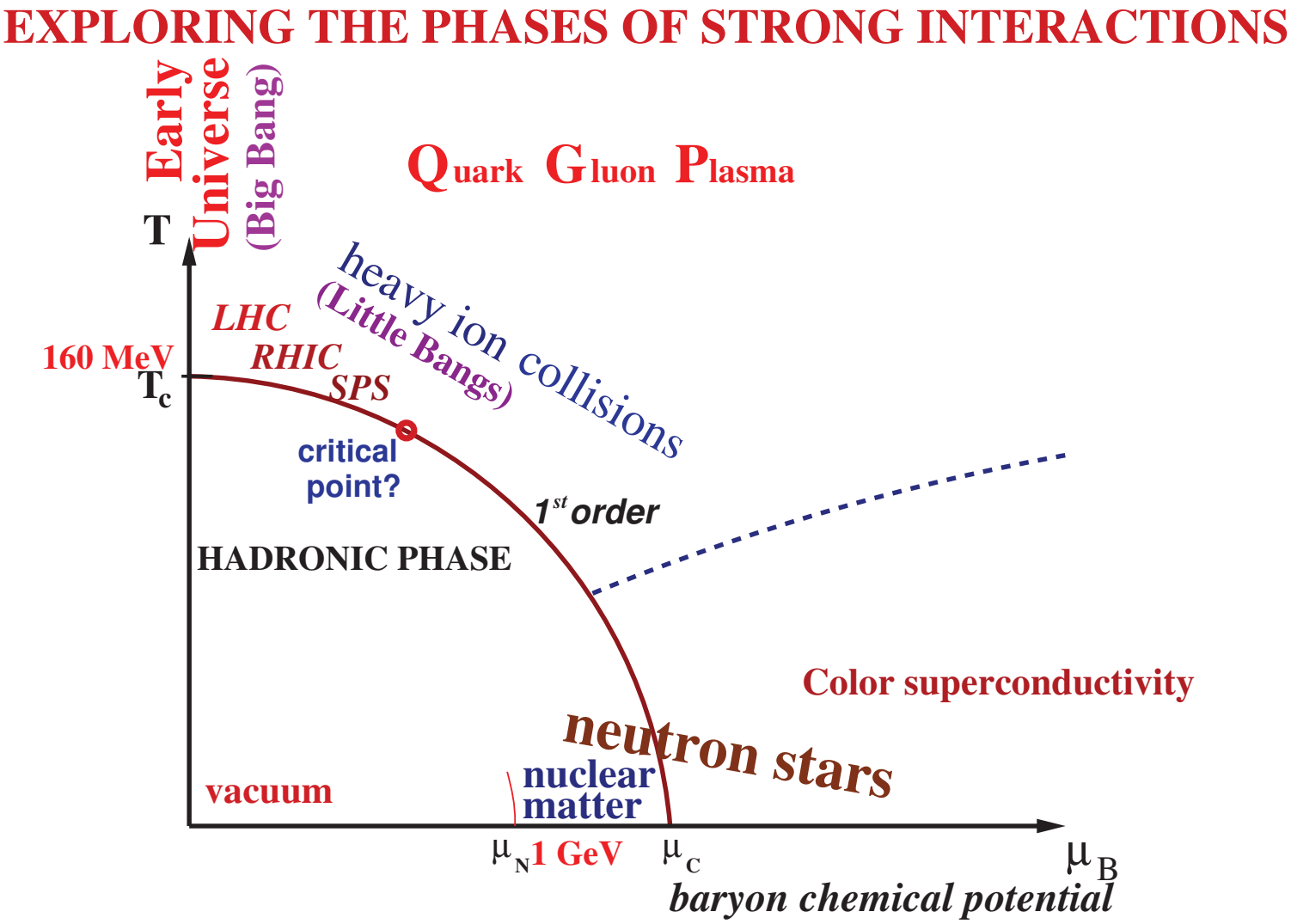


Figure 2: Phase diagram of QCD at high density/temperature, showing the various phases in which hadronic matter organizes.

EPOS, a distributed Infrastructure for solid Earth sciences: the Italian challenge to build this European initiative

The European Plate Observing System (EPOS) relies on a scientific vision and approach in which innovative multidisciplinary research is made possible for a better understanding of the physical processes controlling earthquakes, volcanic eruptions, unrest episodes and tsunamis as well as those driving tectonics and Earth surface dynamics. EPOS is a long-term plan to facilitate integrated use of data, models and facilities from mainly distributed existing, but also new research infrastructures, for solid Earth science. The aim is to obtain an efficient and comprehensive multidisciplinary research platform for the Earth sciences in Europe.

EPOS is integrating the diverse, but advanced European Research Infrastructures for solid Earth Science, and is building on new e-science opportunities to monitor and understand the dynamic and complex solid-Earth System. EPOS is identifying existing gaps and is promoting implementation plans with environmental and space science to help solve the grand challenges facing the Earth and its people.

The Earth Science community worldwide has already begun to reap the benefits of integrated accessible data. The study of solid Earth is necessarily multidisciplinary and requires the access to data and products generated by different communities with different data formats and processing procedures. The understanding of Earth dynamics and tectonic processes relies on the analysis of seismological data, ground deformations inferred from terrestrial and satellite observations, geological studies, laboratory experiments to investigate the chemical and physical processes occurring at depth. In this framework, the next generation of researchers has to be trained to use multidisciplinary data and prepared to collaborate for cross-disciplinary investigations. This is one of the key challenges of environmental sciences.

EPOS integrates national and trans-national research infrastructures (RIs) for solid Earth Science in order to provide seamless access to national and European data and services. Its integration plan relies on open access to multidisciplinary RIs, data and products for promoting cross-disciplinary and transnational research and to foster scientific, technological and ICT innovation. The creation of a novel e-infrastructure through the integrated core services (ICS) is dedicated to a multidisciplinary community of scientists and associated stakeholders. The EPOS progress will be measured through the actual implementation of the services, by the continued and further engagement of stakeholders as well as by the exploitation of products and services for the advancement of basic science, geo-hazards assessment, risk mitigation and a sustainable management of geo-resources. This will in turn represent the EPOS impact on solid Earth Science for successfully addressing global grand challenges in science and fostering a safe and prosperous society.

The ERIC (European Research Infrastructure Consortium) has been selected by the Governmental Representatives of 18 countries as the EPOS legal model. They decided on October 2014 to host the legal seat of the EPOS-ERIC in Italy at the premises of INGV. In July 2015, the EPOS Board of Governmental Representatives, currently involving 24 European countries has launched the call for selecting the country hosting the Integrated Core Service Central Hub (ICS-C). The hosting country will be selected on March 2016. Italy is participating to this selection by offering to host the ICS-C in Italy at the Cineca headquarters.

EPOS is presently in the Implementation Phase, which consists of the legal establishment of the EPOS-ERIC and the EPOS Implementation Phase (EPOS IP) project. EPOS IP builds on the achievements of the successful EPOS preparatory phase project (EPOS PP).

The project, funded by the European Commission with €18,38 million under Horizon 2020, will be coordinated by the Istituto Nazionale di Geofisica e Vulcanologia (INGV) and involves 46 beneficiaries from 25 countries.

EPOS has been included in the ESFRI (European Strategy Forum on Research Infrastructures) roadmap in 2008 and in the Italian roadmap for research infrastructures on 2011. In 2014 the European Union Competitiveness Council has included EPOS in the list of priority research infrastructures for implementation.

25 COUNTRIES

Austria, Belgium, Bulgaria, Czech Republic, Denmark, Finland, France, Germany, Grecee, Hungary, Iceland, Ireland, Italy, Netherland, Norway, Poland, Portugal, Romania, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey, United Kingdom

4 INTERNATIONAL ORGANIZATIONS

Orfeus, Emsc, Euref, Intermagnet

256 NATIONAL RESEARCH INFRASTRUCTURES

4939 SEISMIC STATIONS

2272 GPS RECEIVERS

464 TB SEISMIC DATA

118 LABORATORIES

828 INSTRUMENTS

Several PetaBytes of solid Earth Science data will be available

Several thousands of **users** expected to access the infrastructure

Once the EPOS integrated services will be operational (2020), this new infrastructure will further facilitate sharing the outcomes of researches, not solely by linking data to publications by guaranteeing data traceability and re-use, but also in convincing scientists to share the products of their researches (that is, the new data products). The impact of this collaborative platform for scientific research is still unexplored. Moreover, the next generation of scientists must be trained in developing data intensive applications and modelling. This has to be promoted by using the new opportunities provided by e-science innovation. Building a research infrastructure as a platform for discovery will facilitate collaborations between Earth and IT scientists. The perspectives guaranteed by this federated approach to science have a global relevance and an impact going beyond the scientific community.

Different Italian organizations participate to EPOS. The EPOS-Italia Team includes national research institutions, universities, center of competence, consortia and foundations performing research in all the diverse fields in the solid Earth domain. Besides INGV the other current components are: Cineca, the Italian supercomputing facility, providing e-infrastructure and ICT expertise; the Institute for Environmental Protection and Research (ISPRA), providing expertise in the fields of geology, geological survey and environmental science; the National Research Council (CNR) carrying out research activities in various fields within EPOS, as satellite Earth observation, geothermal energy, geology geochemistry, e-science, experimental facilities for Earth sciences; the National Institute of Oceanography and Experimental Geophysics (INOGS) providing expertise in the field of geodesy and seismology; several important universities, the Universities of Trieste, Genoa, Roma Tre and Naples "Federico II", managing monitoring research infrastructures and experimental facilities of interest for EPOS; the center of competence in the field of Analysis and Monitoring of Environmental Risk (AMRA), providing expertise in this specific field; the European Centre for Training and Research in Earthquake Engineering (EUCENTRE) foundation, a non-profit organization contributing in training and research in the field of seismic risk.

The EPOS-Italia Team has participated in the architectural design since the very beginning. In particular INGV coordinated the EPOS Preparatory Phase providing relevant contribution also by the number of research infrastructures and facilities declared in the Research Infrastructures Database for EPOS (RIDE, http://www.epos-eu.org/ride).

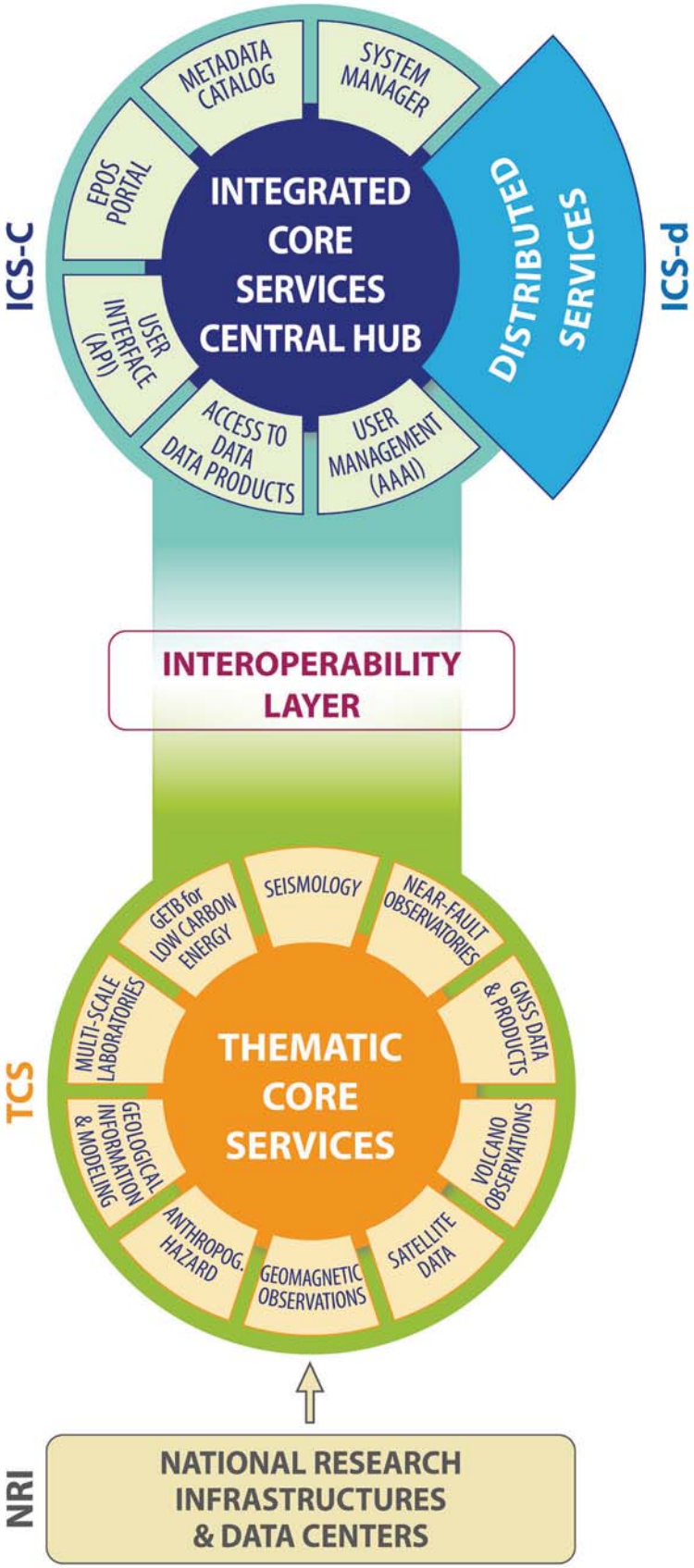
The whole EPOS-Italia Team is participating to the EPOS Implementation Phase and is presently in the process of creating a Joint Research Unit (JRU) to facilitate the participation to the EPOS enterprise that:

"Through the integration of data, products and labs, will enable the international scientific community to develop new ideas and tools to address, in an increasingly accurate way, the challenges concerning environmental risks and sustainable exploitation of the environment and its resources".

From a national perspective, the Italian scientific community considers EPOS as a successful European initiative that will help the coordination of Italian research infrastructures for contributing to structure the national research system in solid Earth sciences. EPOS is a timely initiative responding to the current European need for a comprehensive and integrated solid Earth research infrastructure.

Besides the beneficial impact for both government and industry sectors, private stakeholders will be integrated into EPOS. Several participants in the consortium have a long-lasting and proven experience in working closely with industry sectors concerning hazard assessment (re-insurance), energy (geothermal activities and gas storage) and environment. This will ensure the exploitation of the results and will represent an opportunity for involving private stakeholders. An integrated, coordinated and distributed e-infrastructure represents the best solution to guarantee long-term sustainability, data availability and optimal data analysis for a broad user community including Earth scientists and stakeholders from public and private sectors.

Massimo Cocco
INGV Director of Research and EPOS coordinator



The EPOS architecture is composed by three connected technical and organizational elements: National Research Infrastructures (NRI), generating data and information and responsible for the operation of instrumentation in each country; Thematic Core Services (TCS), the community-specific integration (e.g. in seismology, volcanology or geodesy); Integrated Core Services (ICS), representing the novel e-infrastructure allowing access to multidisciplinary data, products and tools to different stakeholders (i.e. users). The technical interface between TCS and ICS is the interoperability layer. The Integrated Core Service Central Hub (ICS-C) e-infrastructure will include the EPOS portal and its key functionalities: the Access Programming Interface (API), the metadata catalogue, the system manager and the services that will allow the data discovery, the interactions with users as well as the access, download and integration of data. The ICS-C will also provide access to distributed resources, which form the distributed ICS (ICS-d) and will include access to supercomputing facilities as well as to visualization, processing and modelling tools. The ICS-d are currently under design and will be integrated in EPOS through procurement policies to identify existing computational resources at European and national framework.

A life-science challenge: toward realistic models of biological membrane environments for protein simulations

Under physiological conditions, the individual components of biological membranes tend to cluster into distinct domains according to their physicochemical properties.[1] These domains include the so-called lipid rafts,[2] wherein an increasing number of membrane proteins are found to be preferentially partitioned.[3,4] A crucial feature of lipid rafts is a cholesterol-induced coexistence of phase-separated fluid domains.[5] In general, lipid membranes are in equilibrium between two lamellar phases, the gel (or $L\beta$) and the liquid-disordered phase ($L\alpha$). While the gel phase is characterized by translational and conformational order of lipid chains, the biologically relevant $L\alpha$ phase is disordered. Such a behaviour is reflected by a two orders of magnitude difference in the lateral diffusion coefficient (10^{-9} and 10^{-7} cm^2 sec^{-1} for $L\beta$ and $L\alpha$, respectively).[6] The temperature at which a phase transition occurs (melting temperature, Tm) mostly depends on the chain length and saturation of lipids. In this context, cholesterol (Chol) displays a condensing effect on fluid $L\alpha$ phases (above their Tm) and a fluidizing effects on membranes in the $L\beta$ phase (below their Tm). In ternary mixtures containing high and low melting lipids, Chol has the ability to form the so-called liquid-ordered phase (L_o) which is characterized by chain order and an intermediate diffusion coefficient ($D \approx 10^{-8}$ cm^2 sec^{-1}).[5,6] It is nowadays recognized that lipid rafts are represented by a L_o phase floating and diffusing in the surrounding $L\alpha$ phase.[1]

Although membranes used to be considered as passive solvents, it is currently widely accepted that lipids have biological functions and play a key role in several processes. Protein conformational equilibrium, signal transduction, and membrane trafficking are examples of biological events that are modulated by the lipid composition of the membrane.[7] By preferentially interacting with lipids belonging to the raft phase, proteins can support the assembly of the raft itself.[8] From this standpoint, building realistic membrane models able to reproduce structural and dynamical properties in agreement with recent lipidomic data, is a fundamental requirement to achieve a better description of protein-membrane systems through simulations.

According to established models, lipid rafts have been regarded as membrane patches enriched in sphingolipids (SLs), saturated phosphocholine derivatives (PCs) and Chol. However, the optimization of extraction procedures pointed out the presence of phosphatidylethanolamines species, challenging such conventional model.[9] In line with latest lipidomic evidences, we devised a general purpose coarse grain (CG) model for raft bilayers characterized by the presence of lipid species representative of both the outer and the inner leaflet of biological membranes. Specifically, we assembled a three component bilayer containing Palmitoyl-oleoyl phosphatidylethanolamine (POPE), Di-stearoyl phosphatidylcholine (DSPC) and Chol at three different molar ratios with the MARTINI force field v2.0.[10,11] MD simulations were performed with Gromacs 4.6[12] with a time-step of 20 fs. Temperature and pressure were controlled using the Berendsen weak coupling algorithm.[13].

To investigate the effect of the sterol on lipid properties, three raft-like membranes with an increasing amount of Chol were built. These final systems were obtained from homogeneous patches generated with a self-assembly protocol[14] and contained 218, 204 and 192 DSPC molecules. Thus, 90, 76, and 64 DSPC lipids were replaced with POPE molecules in the three patches. In this way, each system contained the same amount of DSPC molecules, which mimics the major lipid components (SLs and PCs). Then, 38, 52, and 64 Chol molecules were introduced, and the systems were further equilibrated. The final molar ratio was 15, 20, and 25% of Chol. These ratios were chosen so as to facilitate lipid mixing,[15] and also because of known condensing effect at these concentrations.[16] By replicating the patches, the final systems consisting of a total number of 1024 lipids each, were obtained. Each system was simulated for 10 μs at the nominal temperature of 300 K. In Figure 1, a pictorial representation of the Chol25% system is reported.

The systems were validated for their ability to reproduce structural and dynamical experimental observables. In particular, concerning structural properties, in systems Chol15%, Chol20%, and Chol25%, average DSPC areas constantly decreased with values of 56.9 ± 0.5, 54.4 ± 0.6, and 51.9 ± 0.5 $Å^2$, respectively. These values properly match with those obtained from atomistic simulations of pure DSPC bilayer [17] and experiments.[18]

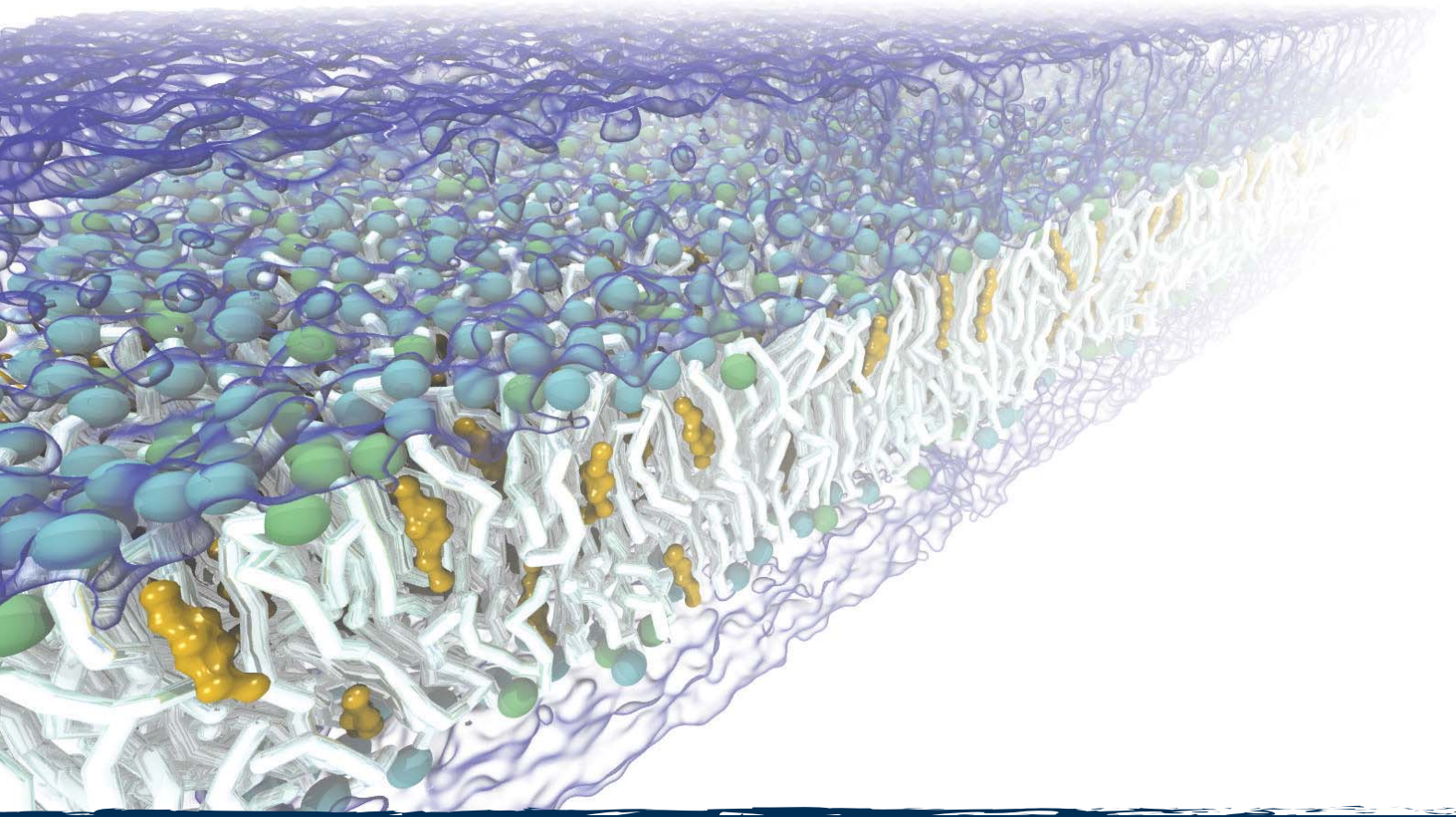
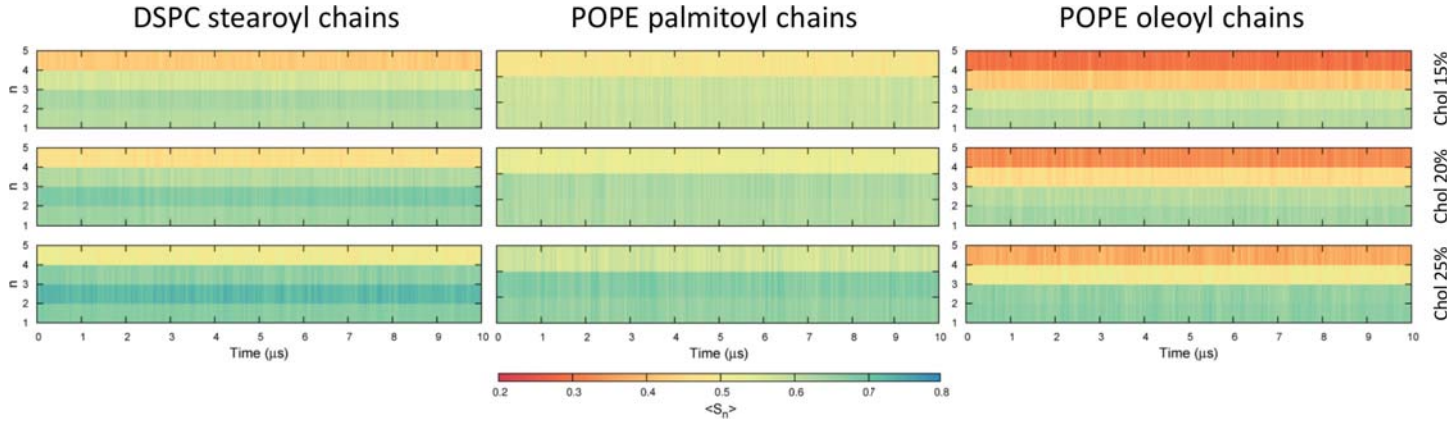


Figure 1: Pictorial representation of the membrane model at 25% in Chol. DSPC and POPE are represented as sticks with a blue and green bead, respectively. Chol is represented as an orange surface.

Figure 2: Deuterium order parameter calculated for the lipid tails of DSPC and POPE plotted against time. Low values indicate increased conformational disorder along the membrane normal.



Analysing the same parameters for POPE, we found average values of 53.4 ± 0.7, 51.1 ± 0.8, and 49.0 ± 0.8 Å^2 for Chol15%, Chol20%, and Chol25%, respectively, in good agreement with experimental values obtained for POPE monolayers in the presence of 30, 40, and 50% of Chol.[16] An interesting feature of density profiles is the increase in Chol density in the middle of the leaflets going from system Chol15% to Chol25%. Moreover, a non-null Chol density in the centre of the membrane was found, reflecting either the ability of this sterol to switch from one side of the membrane to the other, or a certain degree of interdigitation in the inter-leaflet region of the bilayer (or both). Indeed, each system displayed a remarkable ability to exchange Chol molecules between leaflets, while maintaining, on average, a balanced distribution. As a whole, we counted 925, 894, and 711 complete flip-flop events for Chol15%, Chol20% and Chol25%, respectively. As shown in Figure 2, a marked increase of the order was also found going from Chol15% to Chol25% system, for both saturated and unsaturated lipids. We also noticed that a comparable effect was experienced by saturated stearoyl/palmitoyl chains, whereas a less pronounced ordering was found for the POPE unsaturated oleoyl chain. Concerning dynamical properties, the MSD was calculated for the two phospholipids and Chol for the three simulated systems. The decrease in MSD observed for phospholipids and Chol going from system Chol15%, to Chol25%, clearly highlights a progressive reduction in lipid lateral mobility. In spite of this, a fluid behaviour was maintained by all the systems, as reflected by their lateral diffusion coefficient.

In summary, we developed a general purpose CG raft-like model, which was subsequently utilized to simulate membrane systems. We showed that, through a careful selection of lipid components, a homogeneous L_o phase was obtained and preserved throughout 10 μs of CG-MD simulations. The agreement between structural and dynamical properties with those reported for biologically relevant L_o phases makes it an advanced model able to reliably capture the salient features of lipid rafts in computer simulations. Moreover, because of its CG nature, the model is particularly suited to generate complex protein-membrane systems through a simple self-assembly protocol, as shown in Figure 3. This setup-strategy can be conveniently combined with a back-mapping procedure to recover an atomistic description whenever required.[19]

Andrea Cavalli
University of Bologna - Department of Pharmacy and Biotechnology
CompuNet, Istituto Italiano di Tecnologia

Matteo Masetti, Maurizio Recanatini
University of Bologna - Department of Pharmacy and Biotechnology

Mariarosaria Ferraro, Giovanni Bottegoni
CompuNet, Istituto Italiano di Tecnologia

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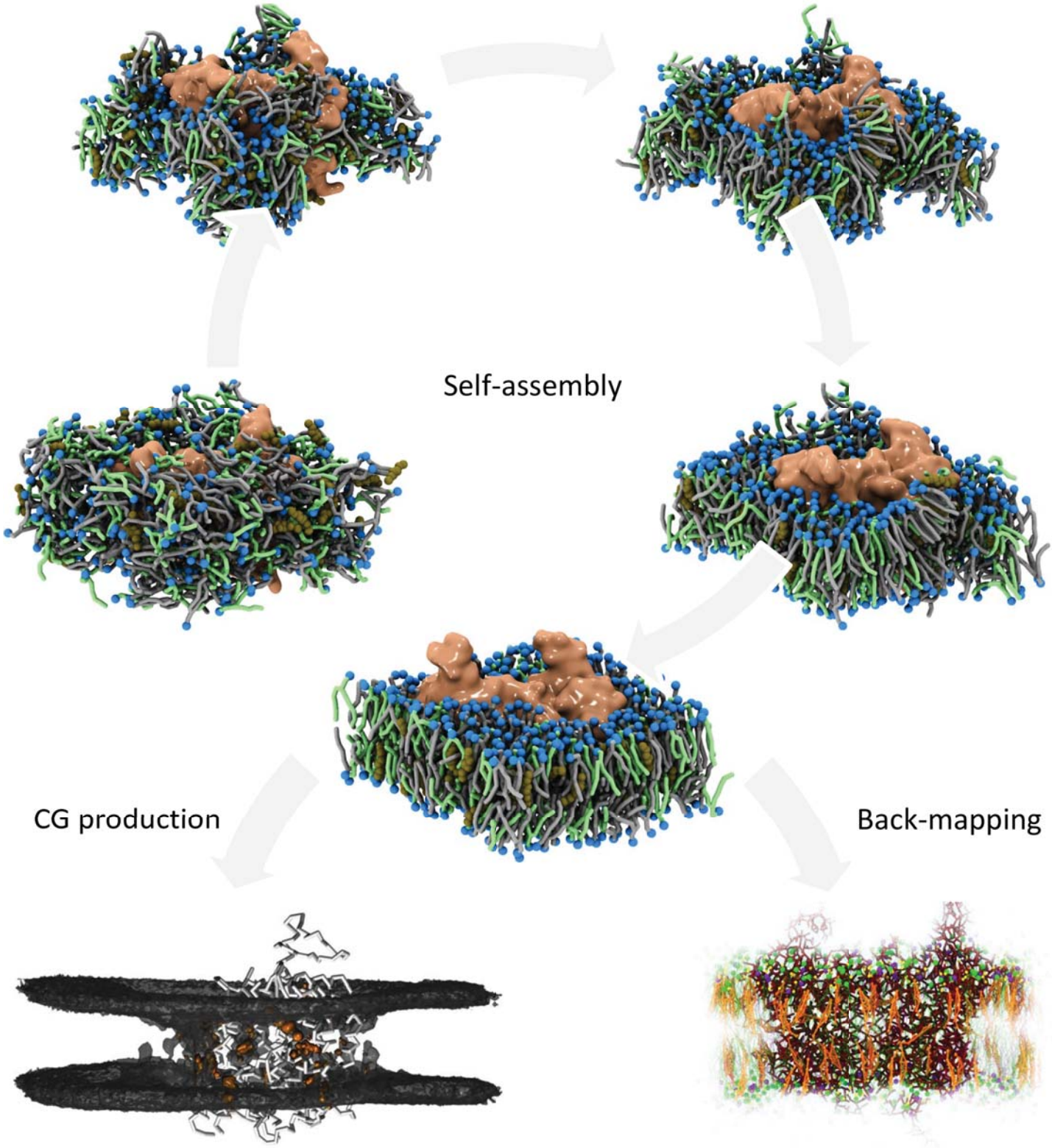


Figure 3: Snapshots taken from a typical raft-membrane self-assembly simulation. As the Figure shows, during the course of the simulation, the originally random distribution of lipids in the simulation box is progressively adapting to the protein surface. At the end of the process, a protein-embedded lamellar membrane is obtained, and the system is ready for CG production, or alternatively, to be back-mapped into a fully atomistic representation.

Section 3: 2015 HPC in numbers; assessment and impact

2015 HPC in numbers: use & users of our infrastructure

Our access policy and resource management

Starting from July 2010 and starting up the first round of ISCRA projects, Cineca has deeply revised its policy for access and resource management on HPC machines.

Access to HPC platforms is allowed to "login" owners, this meaning that each user is uniquely identified by a username/password pair. Login credentials are to be considered as strictly personal, no sharing between members of the same working group is expected to happen. Each single user entitled with login credentials is to be considered personally responsible for any misuse that should take place.

Users will keep their login credentials as long as they work on Cineca platforms such that a personal usernames' life is not bound to specific projects the user is involved in.

Relevant information related to projects, such as budget in CPU-hours, assigned host and dates for their beginning and end, are managed within the scope of the PROJECT (also called ACCOUNT): this is defined for each single project (e.g. approved ISCRA or PRACE projects and similarly for internal accounting centers provided with budgets and lifetime). One or more users, once provided with login credentials, can be associated to one or more projects, also in a concurrent mode: an individual user could be the Principal Investigator for one or more projects, and could also wish to join others projects as a collaborator. Users associated with at least one project can submit jobs to the resource manager in batch mode, by specifying which project budget is to be billed for job execution.

The preferred entry point both for users and projects remains our UserDB, a web-based application where users can register, ask for services, manage their resources, submit applications to our allocation programmes and so on. UserDB is available at userdb.hpc.cineca.it or via our HPC portal (www.hpc.cineca.it).

Our users

During the year 2015, we acquired about 200 new users for our HPC systems, the total number increasing from 1.689 to 1.877.

The registered users in our DB exceed 2.500 but only 1.877 are actively accessing the HPC resources, some accounts being expired (no access for more than one year) and some others never finalizing their enrollment.

Not surprisingly, the great part of our users are males and Italian (79% and 78% respectively)(see Figure 1), a figure substantially unchanged with respect to last year (81%). The youngest user is 21, the oldest 83 with a mean age of 38.

Among the more popular foreign nationalities: France and Germany, followed by Spain and United Kingdom, but also India and China are well represented (see Figure 2).

83% of our active users belong to an Italian Institution, mainly to a University, as reported by Figure 3.

The large Italian cities, aggregating several Research Institutions, are well represented: 339 users come from Milan, 304 from Rome, 158 from Trieste (University, Sissa, ICTP, OGS), 98 from Bologna, 70 from Modena and 67 from Turin (see Figure 4).

As one might expect, the great majority of the users are scientists: Chemistry and Condensed Matter Physics are among the more traditional and populated disciplines. Computational Fluid Dynamics is very represented, thanks to emerging algorithms that are well suited for the new HPC architectures. New entries in the list are Mathematics (and Computer Science) and Humanities and Social Science, this latter including researchers involved in the new BigData infrastructure (see Figure 5).

Allocation programmes

The computational resources are mainly distributed by means of peer-reviewed allocation frameworks at different levels: regional for Regione Lombardia (LISA), National (ISCRA) and European (PRACE). Researchers can submit their projects to the frameworks with calls proposed twice a year. After a technical check by the internal staff and a scientific peer-reviewed evaluation by a scientific committee, the best proposals are selected and given access to the most advanced computational resources available worldwide.

During 2015 (from Nov the 1st, 2014 to Oct the 31st, 2015), a total of 1,272 billion core-hours has been distributed on the Tier 0 machine (Fermi). 808 million core-hours was awarded to PRACE projects and 435 million to ISCRA (also 24 million for agreements, 2M for EU projects, 1 M for trial projects).

Figure 4: Cities of the Cineca users Italian institutes

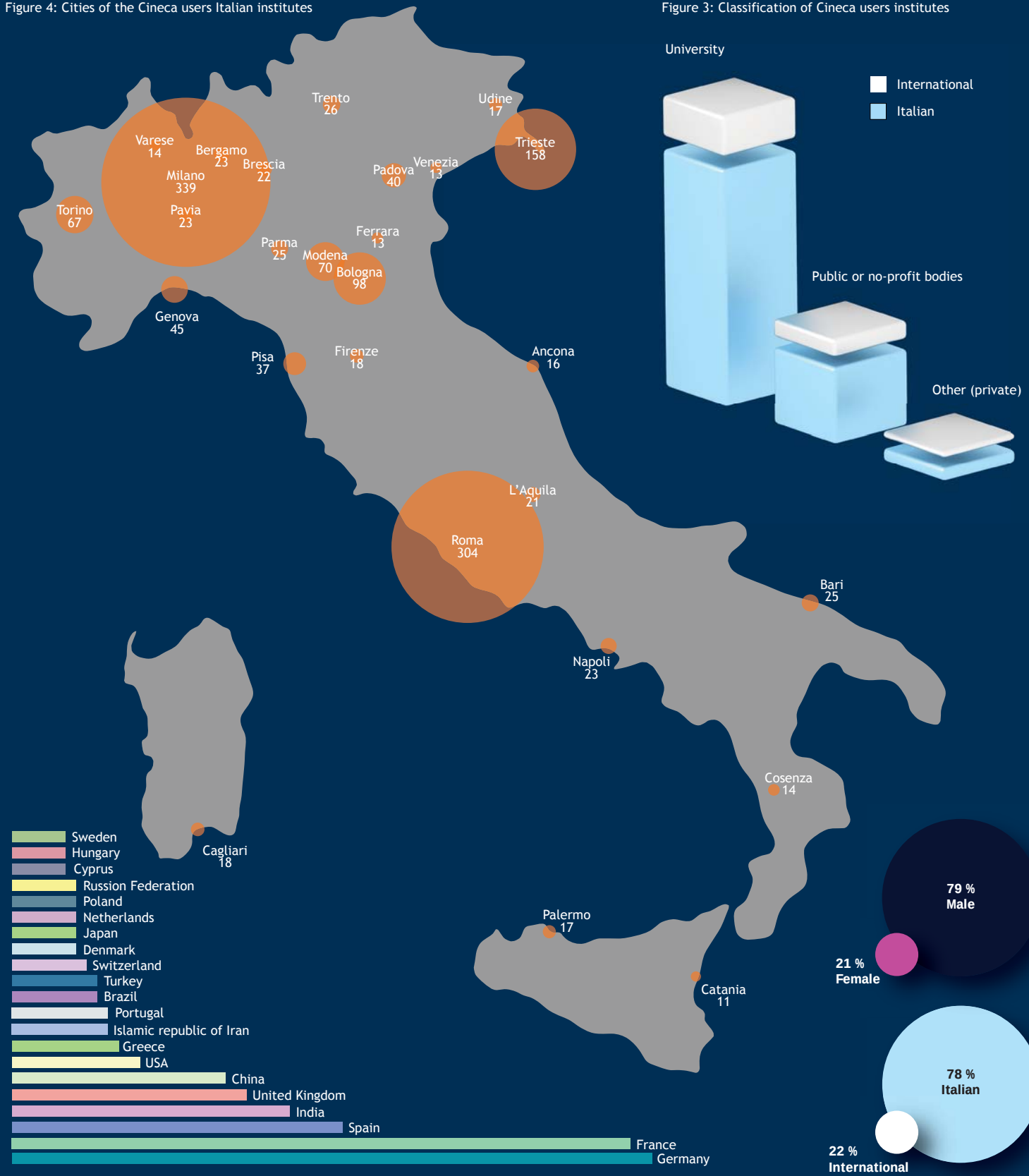


Figure 3: Classification of Cineca users institutes

Figure 2: Nationalities of Cineca users

Figure 1: Number of Cineca users divided by gender and nationality

In the same period, a total of 57 Million Core-hours has been distributed on Galileo: 37 million was awarded to ISCRA projects and 0,5 million to PRACE (0,5 M innovation, 1 M EU projects, 17 M agreements).
The LISA regional Programme has been suspended during 2015: the last call was in May 2014 and will be resumed in Dec 2015.
In Figure 6 the distribution of computational resources with respect to the allocation programs are reported.

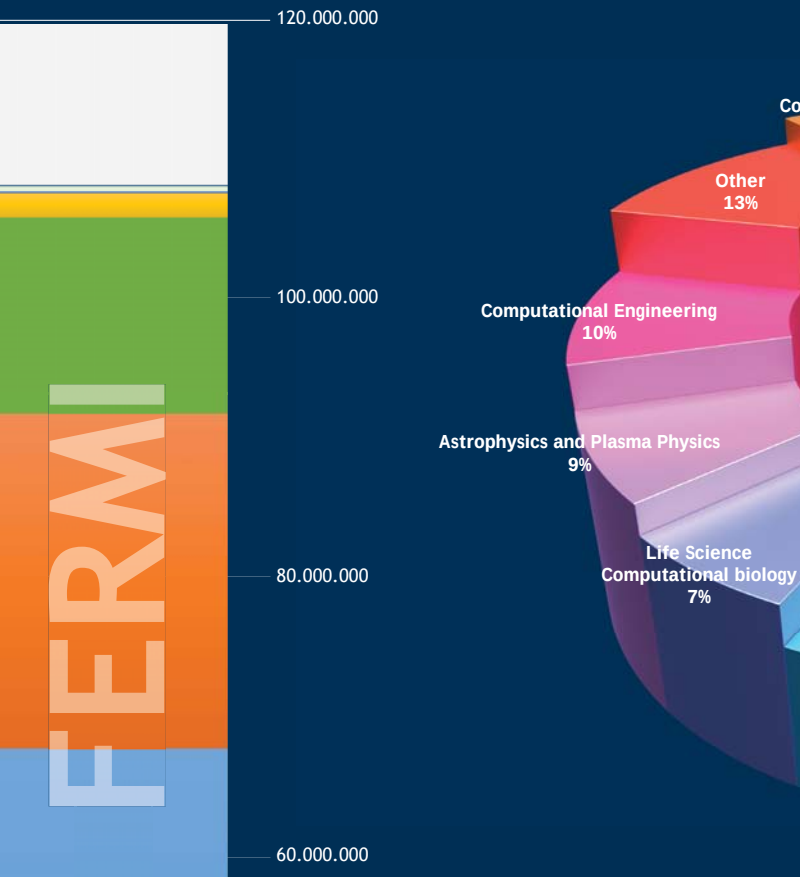
How computational resources have been used

The two main HPC systems in Cineca are very different in capacity. Fermi is a 160 thousand cores system with a total capacity of 1.5 billion core-hours per year. Galileo (in its research partition) is a 6784 cores system with a total capacity of 60 million core-hours per year.
Both systems have been fully exploited during 2015, even if it should be recalled that Galileo entered in full production only in spring 2015.
Fermi reports a global use percentage greater than 90%, and Galileo 95%.
In Figure 7 a monthly avarage distribution is reported for Fermi and Galileo.

The User Support

Cineca puts a strong effort in the support of the users. This has always been for us a crucial task for assuring an effective service for the research community. A number of professionals, trained in technical and scientific topics are working within a schedule to ensure the Help Desk presence during working hours. The support is operated through a Trouble Ticketing system available via email (superc@cineca.it).
The Help Desk service is governed by a ISO9001:2008 procedure, for the quality management, defining the process with KPI (Key Performance Indicators) and related target values, such as all tickets must be taken into consideration within a working day.
During 2015 (from Nov 2014 to Oct 2015) a total of 2510 contacts were received, reporting problems (40%), service requests (30%) and information requests (30%). The average time for taking the request into account was less than one hour, with a descending trend over time.
One of the tasks of the Help Desk team is the installation of applications, tools and libraries on the HPC systems. This is done within the “module” framework, assuring the simple and easy access to common tools. All the software applications available are described in our web site (www.hpc.cineca.it/content/software) and a comprehensive documentation on their use is available on the HPC platforms.
Tools for developers are available (compilers, libraries, debuggers, profilers) as well as scientific applications spanning different scientific fields: Chemistry, Physics, Life Science, Bioinformatics, Engineering, Astrophysics, etc.
On each system the best suited applications are pre-installed, for example on Fermi the user can find only applications with a very good scaling behavior, while Galileo hosts more general applications.

Figure 7: Core Hours production on Fermi (Tier 0) and Galileo (Tier 1) in 2015, on a monthly base.



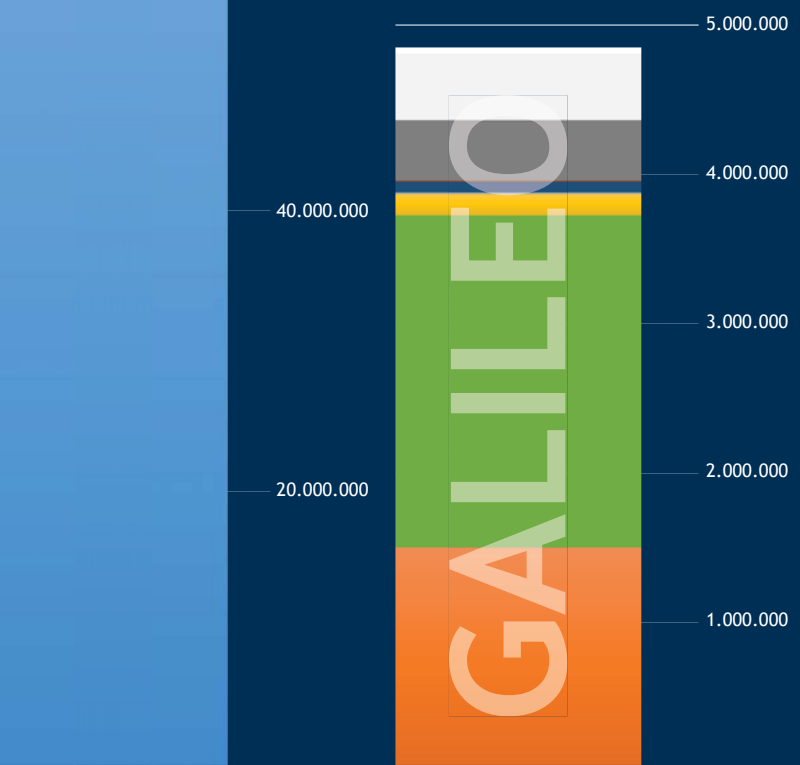


Figure 5: Research area of Cineca users

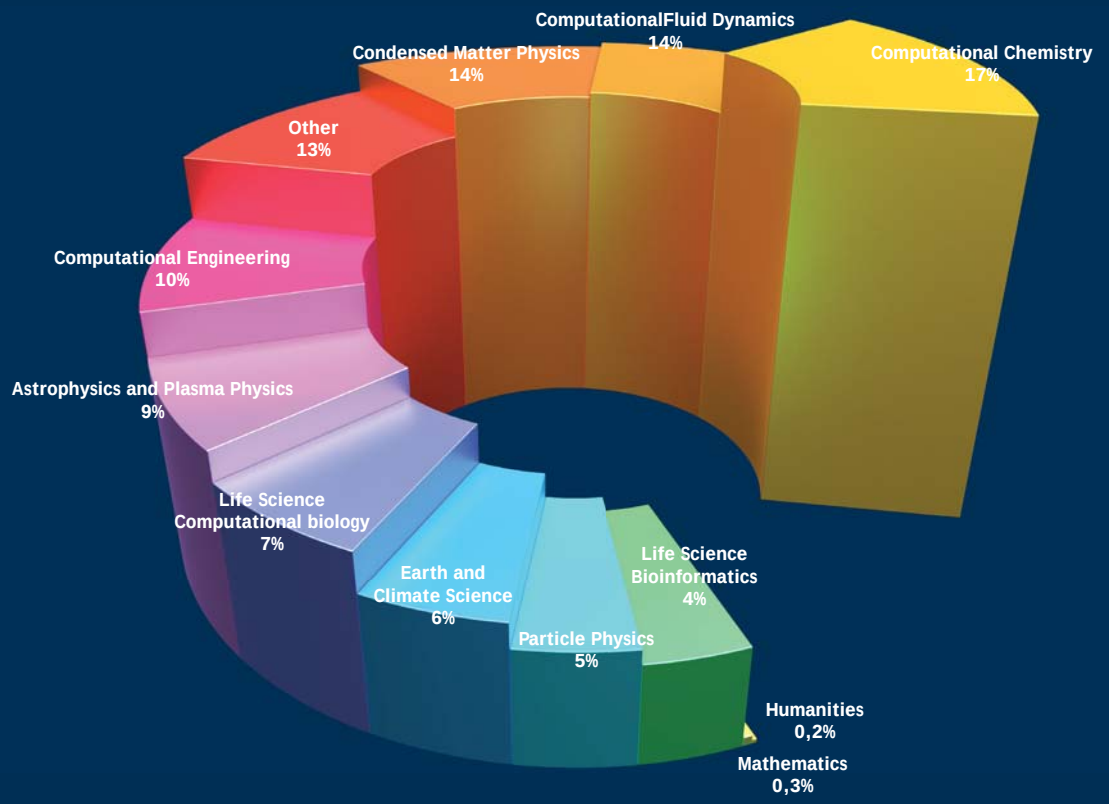
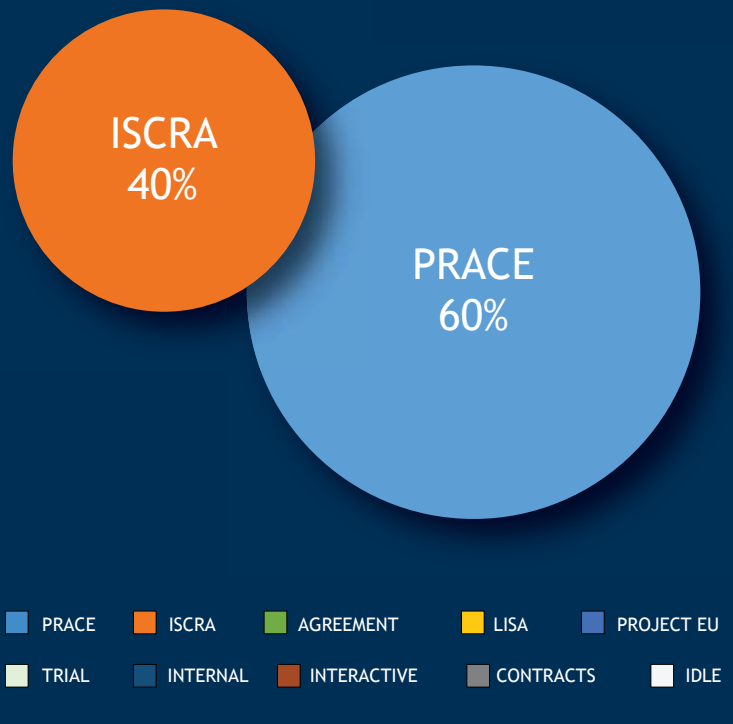


Figure 6: Distribution of core hours on HPC infrastructures via call PRACE, ISCRA, LISA.



Training

Training has always been a hallmark of the support activities carried out by Cineca for the Italian research community and users. Starting from 2012 it was extended to European researchers, Cineca being recognized as a PRACE Advanced Training Center in HPC.

During 2015 we reached quite impressive numbers: 18 courses, distributed in 31 different editions, held in the three sites of the consortium, Bologna, Milan and Rome; 3 schools in 4 editions and 2 workshops. 50 people in the SCAI Department contributed as teachers, for a total of 150 days of lectures and highly specialized training.

In total, by 30th September 2015, over 700 Italian and European researchers had benefited of our training program and by the end of the year students will exceed 850, increasing the 2014 figures by 20%.

Students appreciate these courses and the surveys show high satisfaction levels, reporting an average rating of 8.5/10.

In addition, teaching collaborations have been activated in 3 academic courses (Masters and Doctorate schools), held in some Italian Universities.

Besides traditional lectures, many other initiatives attracted very young promising scientists to Cineca, to spend short or extended visits under the mentoring action of our experts, who help them to maximize the output of their research or enhance their expertise in HPC techniques.

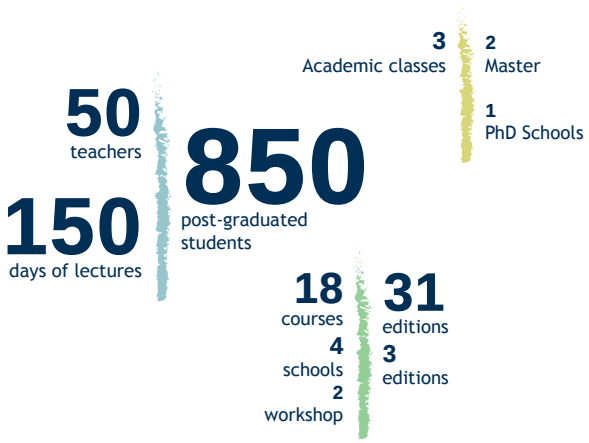
Also this year we took part in Summer of HPC (SoHPC), a PRACE initiative offering young University students from all over Europe the chance to do internships at major computer centers in Europe in the months of July and August. In summer of 2015 we hosted two students: Cem Benar who worked on “Visualization Tool for Olfactory Bulb Data” and Leon Kocjancic on “Exploring Mars Surface”. The resulting videos are available on YouTube (search for SoHPC 2015).

Elda Rossi, Claudia Truini
Cineca

Numbers:
18 courses (31 editions) (11 Courses PATC)
including:
3 schools (4 editions)
2 workshops

50 Cineca teachers
150 days of lectures
100 hours in Academic classes
850 students

3 Academic classes (2 Master e 1 PhD Schools)



Cineca
COURSES
High Performance
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CINECA SCAI
SuperComputing Applications and Innovation

PRACE

Cineca offers every year a deep and solid teaching program in the field of Scientific Computing, to guarantee a reliable support to scientists who need an advanced training to compete in their specific research field.

24th Summer
School on
PARALLEL
COMPUTING

25 May - 5 June, 2015
Cineca - Bologna

13 - 24 July, 2015
Cineca - Rome

CINECA SCAI
SuperComputing Applications and Innovation

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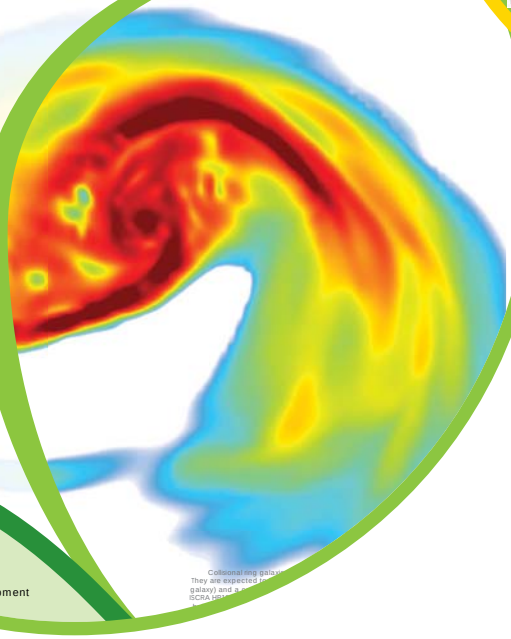
11th Advanced
School on
PARALLEL
COMPUTING

9 - 13 February, 2015
Cineca - Bologna



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PRACE

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HPC architectures evolve and enhance computational science

In the 30 years from when the first vector supercomputer (Cray XMP12) was installed, Cineca has had the objective of accelerating scientific discovery by supporting the Italian and European research communities in providing a world-class HPC and data infrastructure. Currently SCAI, the Cineca HPC and data analytics department, is driving the procurement process for Marconi, the new Tier 0 system which will replace Fermi the current Tier 0 system with a peak performance of 2 PFlop/s. In mid 2016, Marconi is expected to be in production and capable of a performance in excess of 10 PFlop/s.

In June 1993, when the first edition of the Top500 list of the world's most powerful supercomputers appeared, the system in the 1st position (a CM5 with 1024 cores installed at LANL) had a performance of 131 GFlop/s. In the same list, the Cineca Cray YMP supercomputer was ranked in position 226 with a peak performance of 1.3 GFlop/s. In the current list (November 2015) the world's No. 1 HPC system is the Tianhe-2, a Intel Xeon cluster developed by China's National University of Defense Technology, equipped with 3,120,000 cores, 54.9 PFlop/s and a power consumption of 17.8 MW. In the same list Cineca's Fermi system holds the 37th position.

Ever since the first publication of the Top500 list, Cineca has held a stable presence in the Top 500 list, with at least one system (Figure 1). The highest positions have been reached in November 1998 (Cray T3E, rank 38) and June 2012 (BG/Q, rank 7). Overall, the trend in performance of the Cineca HPC systems has been a linear evolution in line with those of the major HPC sites world-wide (Figure 2).

Since 1993, there has been a million-fold increase in performance of Cineca's HPC systems. In this long period, Cineca has always been always able to exploit to the full the evolution of the architectural paradigms, for the benefit of the Italian scientific community: the first vector supercomputer was installed in 1985 (Cray XMP) and the first parallel supercomputer arrived in 1994 (Cray T3D); Cineca reached one TFlop/s performance in 2002 (IBM SP4), 10 TFlop/s in 2006 (BCX IBM Cluster linux), 100 TFlop/s in 2009 (IBM SP6) and two PFlop/s in 2012 (BG/Q Fermi).

A new HPC trend in computer architectures started around 2005 when multi-core chips began to emerge on the market, representing a good option for application scalability, beyond traditional CPU implementations. Following the general trend in HPC and acceleration adoption ninety-eight percent of the systems in the 2015 Top 500 list use processors with six or more cores, and more than one hundred systems now incorporate accelerator technology. The Cineca HPC systems are well aligned with this trend.

The size and resolution of the problems scientists address today are limited only by the size of the data they can reasonably work with. There is a constantly increasing demand for faster processing on bigger data and, clearly, exascale performances will be measured in terms of EFlop/s integrated with EBytes.

In the drive towards exascale, a renewed emphasis on data-centric processing, energy efficiency concerns, and memory and I/O performance will affect the architectural trends: many-core accelerators, flash storage, 3-D memory, integrated networking, and optical interconnects are expected to become the standard technologies for the next HPC architectures.

Figure 3 shows the resources granted on the Cineca systems over the years. The increased availability of resources together with the evolving performances of the HPC systems allow Italian scientists to perform ground-breaking research in different fields. The impact of the HPC service offered by Cineca on the scientific communities and on innovation at large is pointed out by the high number of research papers published by Italian researchers, acknowledging the resources granted by Cineca (Figure 4).

Many examples in different computational fields, from cosmology to material science, from life science to CFD, demonstrate how the evolution and the increased power of HPC architectures allow us to investigate new problems with a realism and complexity unthinkable even a few years ago.

State of the art SPH/TreePM cosmological codes (i.e. Gadget 3) allow us to simulate the whole universe evolution, using the resolution needed to obtain, for the first time, some constraints on the nature of dark matter. These simulations consider tens of billion of particles and run on 32K-64K cores of Fermi, producing several hundred TBytes of data. It should be emphasized that until a few years ago it was possible to simulate only a few galaxy clusters.

Eulerian MHD codes (e.g. Pluto), in solar physics allow us now to finely resolve the structure of solar corona, in order to investigate the nature of the coronal heating mechanism, modeling for the first time the magnetic reconnection inside coronal loops, or studying the evolution of entire active regions.

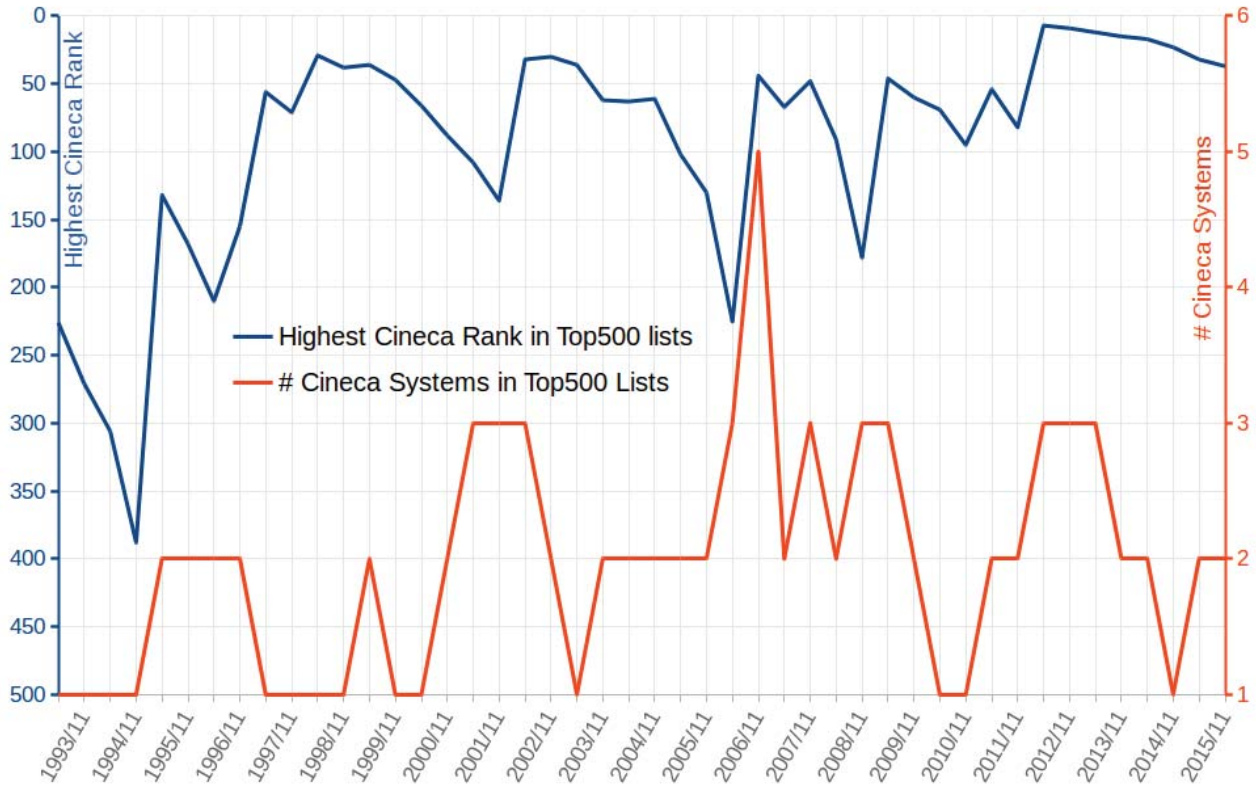
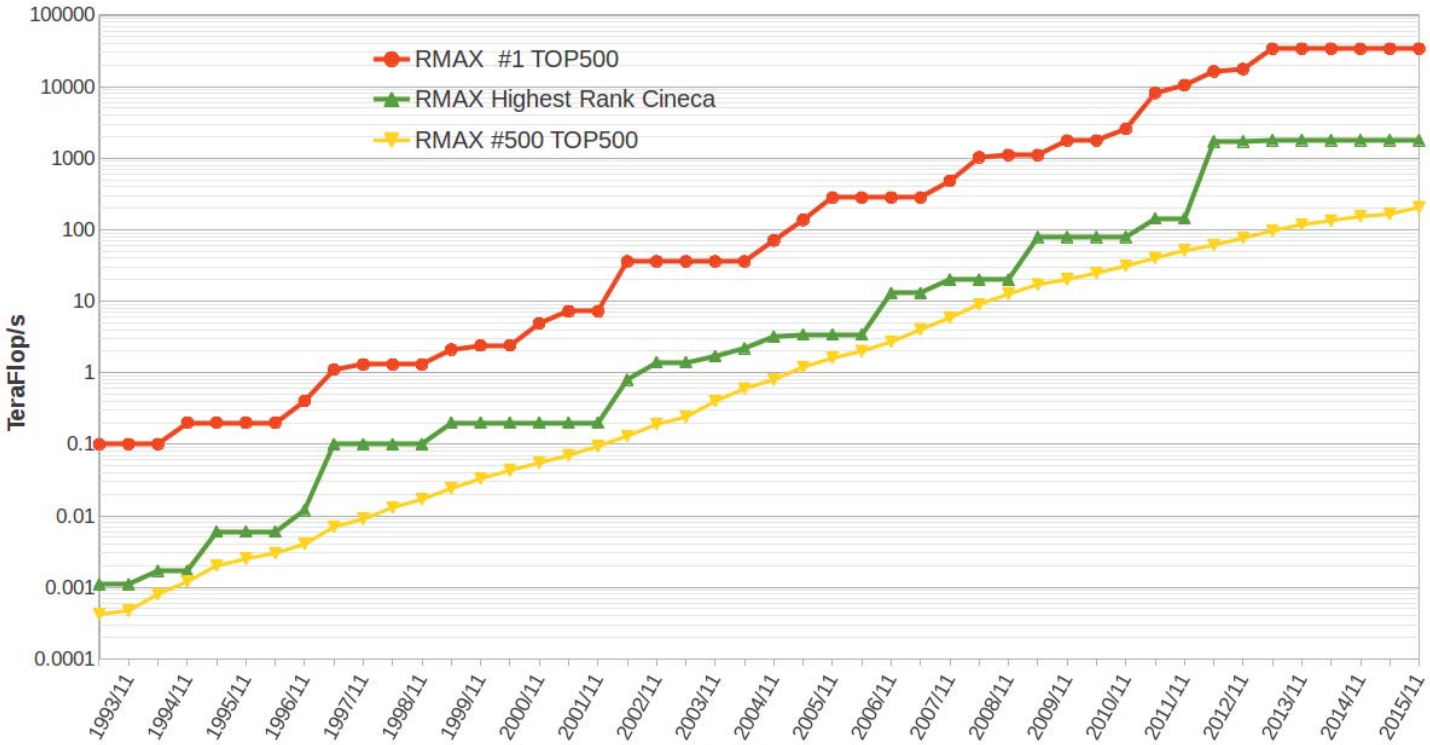


Figure 1: Presence and performance of Cineca's HPC systems in the Top 500 lists (1993 - 2015)

Figure 2: Performance (Rmax LINPACK) of the most powerful HPC system of Cineca in the Top 500 lists (1993-2015) compared with the systems ranked #1 and # 500



This represents a big step ahead compared to simulations of ten years ago where the state of the art involved single loop simulations with simple 2D models, analyzing only some indirect effects of the coronal heating mechanism. Pluto simulations can scale up to 100k cores on 512^3 point grids.

A few years ago, PIC codes (e.g. iPIC3D), allowed us to model only very small plasma systems whereas, with the HPC systems available today and improvements of the code scalability, it is possible to create some very accurate 3D models of the plasma confined in a Tokamak fusion reactor, or to model the interaction of the solar wind with the terrestrial magnetosphere.

The first simulation in molecular dynamics (MD) was performed in 1959, with a system of 500 particles and took two weeks on an IBM 704. Since then, MD simulations have improved impressively. In 2006 the complete MD simulation of the satellite tobacco mosaic virus was reached involving one million atoms for a 50 ns simulation using NAMD on a 128 node cluster, and in 2011, the simulation of a chromatophore involved a structure of 100 million atoms. The trend has been to simulate ever larger atomic systems and at time scales now approaching those involved in many biological processes (e.g. at the microsecond or even millisecond regime). Coupled with improvements in algorithms, particularly enhanced sampling methods such as metadynamics, it is now possible to investigate a wide variety of physical and biological phenomena.

In material sciences, new more accurate algorithms have been recently introduced and are the basis of state of the art simulations (e.g. exact-exchange in DFT). New methods are available, like material screening which allows us to proceed in high-throughput mode to identify physical properties, common to tens of thousands of structures. As an example of application scalability, it is worth mentioning the Yambo code where the scalability has improved from tens of cores (in 2009) to thousands of cores for simulations today.

The 2013 Nobel Prize in Chemistry was awarded to Martin Karplus, Michael Levitt and Arieh Warshel “for the development of multiscale models for complex chemical systems”. It was not only a recognition of the ground-breaking work of these scientists but also a recognition of how profoundly computational modelling has transformed modern research in chemistry, materials science and the life sciences, thanks to the evolution of HPC systems in terms of performance and availability of resources.

Computational Fluid Dynamics (CFD) has facilitated the work of aerospace and mechanical engineers by yielding a substantial reduction in the time spent in wind tunnel testing, but also providing added physical insight, enabling more accurate design at a reduced cost. The range of physical models spanned by CFD is extremely wide, ranging from crude RANS (Reynolds-averaged Navier-Stokes) turbulence models which may run on personal computers, up to direct numerical simulations (DNS) of the full Navier-Stokes equations, which may require several millions of CPU hours on massively parallel computers. Computer power limitations have so far prevented DNS from being applied to real-world problems, as typical applications are characterized by values of the Reynolds number (Re, being a measure of the importance of inertia forces as compared to viscous forces) in the range of 10^6-10^{10}. Since the DNS of homogeneous turbulence requires a number of grid points roughly proportional to Re^3, it is clear that the cost of DNS very soon becomes prohibitive for any current computer, both in terms of memory allocation and of CPU effort.

The current status of DNS can be well understood by looking at Figure 5, which shows the Reynolds numbers reached over the years in the simulation of turbulent channel flow, a standard, widely investigated case to understand the fundamental physics of wall turbulence.

The figure suggests steady exponential growth of the achieved Reynolds number, with the current record at $Re = 3 \times 10^5$. Based on this chart, Reynolds numbers typical of industrial applications are expected to be attained some time around 2035. Besides the obvious importance of getting closer to conditions of practical relevance, the quest for DNS at higher and higher Reynolds number has the important physical relevance of allowing us to sense effects which are not observed at computationally ordinary Reynolds numbers, and which are difficult to measure in experiments.

The innovative architecture of the new Marconi Tier 0 system, together with the availability of significantly larger computational resources, will represent a further step ahead for Italian scientists to reach new scientific breakthroughs.

Giovanni Erbacci
Cineca

Figure 3

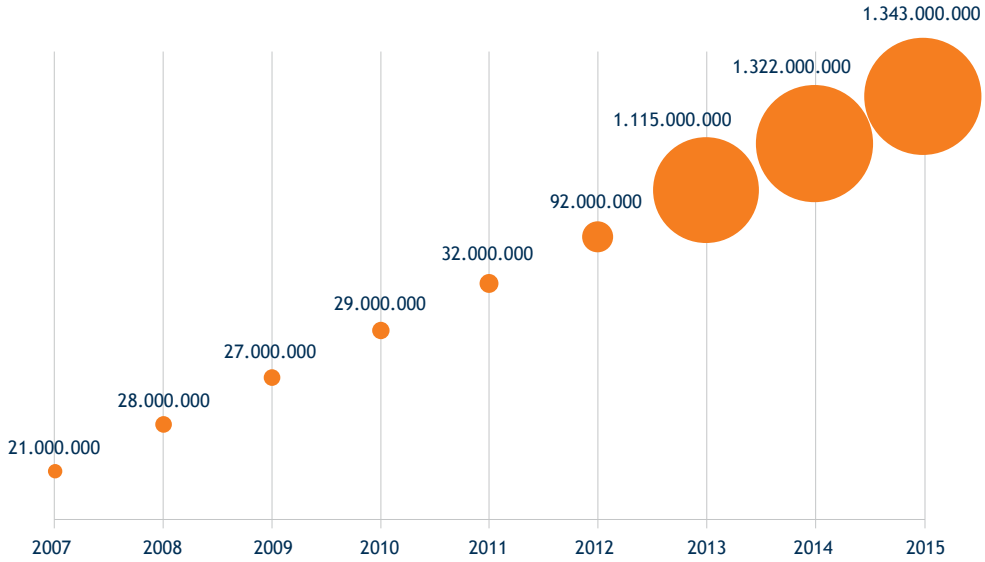


Figure 4

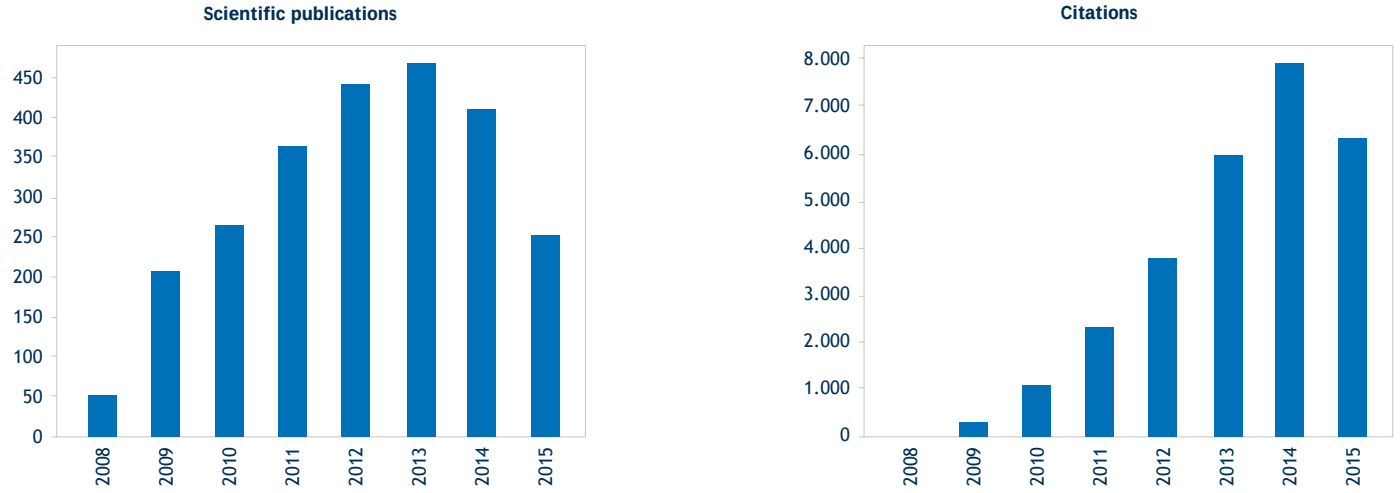


Figure 5

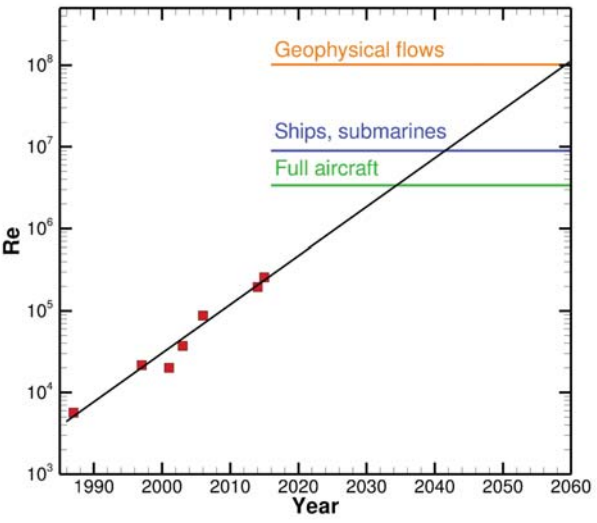


Figure 3: HPC resources (core hours) granted on Cineca's HPC Systems

Figure 4: Number of scientific publications produced by Italian scientists acknowledging the resources granted by Cineca and number of citations.
Information extracted from the reference database "Web of Science", analyzing the publications using HPC technologies in all the science and engineering fields. On a seven years time-span, 2008-2015 (the data of 2015 are incomplete), we got 2465 publications mentioning Cineca as funding source.
97% of all publications have at least one author from an Italian organization. Among the authors coming from foreign countries, the largest part comes from USA (11%) and Germany (11%), France (10%), Spain (7%) and England (6%), followed by Switzerland, Netherlands, Japan, etc.

Figure 5: Reynolds numbers reached over the years in the simulation of turbulent channel flow (Courtesy of Matteo Bernardini University of Roma La Sapienza)

Section 4: Scientific Reports

Presentation of the Users' Reports

The infrastructure of Cineca is accessible according to the three specific allocation channels, PRACE, ISCRA, LISA and, a smaller quota, to development projects and projects related to agreements of joint collaboration between Cineca and outstanding national research entities.
At a national level ISCRA is the major program allocating HPC resource facilities for academics of all disciplines. PRACE allocates resources centrally, at a European level, and Cineca is one of the sites hosting a Tier 0 system included in the PRACE infrastructure.
Both ISCRA and PRACE allocate resources on the basis of a peer-review process. In both cases the selection is based on scientific merit, taking into account originality, innovation potential, scientific excellence, qualification and competence of the proponents, international and national relevance and the match between requested resources and objectives of proposal. No preliminary allocation between disciplines or provenience is made. A rigorous peer-review system is implemented.
A very significant support to researchers is offered by the in-house SCAI experts in all the phases of the research work, in the optimization of the codes, in the testing of their effectiveness and scalability, in the drafting of the proposal, as well as, of course, in the implementation of the research on the systems, for ensuring the best exploitation of the machines. This is in accord with one of the missions of SCAI: that of enabling researchers to attack the scientific challenges of their domain, focusing only on science while benefiting, for all HPC and HPCD matters, from the extensive experience and specialized skills of our staff.
In this 2015 report we are pleased to offer you a selection of the reports that we require each Principal Investigator to provide in order to share and disseminate the outcomes of the research. The articles are from users selected via ISCRA at the national level, and through PRACE at the European level.

Francesca Garofalo
Cineca


PRACE
PRACE
Italian PI
Projects on FERMI
Chemical Sciences and Materials
Biochem. Bioinf., Life Sciences
Earth System Sciences
Engineering
Universe Sciences
Mathematics and Computer Sciences
Fundamental Physics
Fund. Constituents of Matter
Earth System Sciences
Engineering
Biochemistry, Bioinformatics and Life Sciences
Chemical Sciences and Materials
Universe Sciences
Mathematics and Computer Sciences
Fundamental Physics
Fund. Constituents of Matter
Curie 8.500.000
Matteo Ceccarelli, Cagliari University Antibiotics transport through specific porins from Pseudomonas aeruginosa and rules for enhanced permeability
45.416.379 Juqueen 100.000 Curie
Leonardo Guidoni, L'Aquila University Ground state structures and electronic excitations of biological chromophores at Quantum Monte Carlo- Many body green's function theory level
Hermit 11.000.000
Simone Piccinin, CNR-IOM Kinetic model of ethylene epoxidation on Ag surfaces
Curie 35.000.000
Fabio Cecconi, CNR Application of biological nanopores for the detection of protein post-translational modification.
SuperMUC 20.739.000
Jost von Hardenberg, CNR Climate stochastic physics high resolution experiments
SuperMUC 8.000.000
Walter Boscheri, Trento University Lagrangian space-time methods for multi-fluid problems on unstructured meshes
SuperMUC 15.728.640
Bruno Giacomazzo, Trento University General relativistic simulations of binary neutron star mergers
10.000.000
Michele Migliore, National Research Council 3DBULB
17.208.576
David De Sancho, Cambridge University The origin of internal friction in enzyme dynamics
38.000.000
Mariorie Bertolus, CEA, DEN Investigation of the formation of defects, incorporation of rare gases and oxidized phases of UO2 using large supercells
60.600.000
Mathieu Luisier, ETH Zurich Ab-initio simulation of transition metal dichalcogenide devices
23.000.000
Joanne Mason, Exeter University Magnetic field generation in rotating, stably stratified turbulence
50.000.000
Paolo Gualtieri, La Sapienza Roma University Turbulence dynamics in the separation region of channels with lower curved walls
68.550.000
Roberto Verzicco, Twente University Surfing for thermals in turbulent flows
17.860.000
Giannaria Sannino, ENEA Numerical experiment on the Mediterranean model response to enhanced resolution and tide
30.000.000
Aurélien Ponte, Ifremer Modelling interactions between mesoscale, submesoscale and internal tides for high resolution satellite altimetry
55.000.000
Luca Biferale, Tor Vergata' Roma University Effect of helicity and rotation in turbulent flows: Eulerian and Lagrangian statistics
34.000.000
Franco Moglie, Marche Polytechnic University Advanced simulation of loaded reverberation chambers
80.000.000
Thomas Schmitt, EM2C laboratory, CNRS, Ecole Centrale Paris Large-Eddy Simulation of a meso-scale rocket engine with self-sustained combustion instability
29.127.111
Petros Koumoutsakos, ETH Zurich Direct numerical simulations of cloud cavitation collapse in turbulent flows
50.000.000
Alberto Giacomello, La Sapienza Roma University Salvinia-inspired surfaces in action: slip, cavitation, and drag reduction
19.000.000
Stephane Zaleski, Institut Jean Le Rond d'Alembert Modeling of multi-scale interfacial flows
50.000.000
Sergio Pirozzoli, Sapienza, Roma University Control of wall turbulence at high Reynolds number
18.000.000
Silvano Simula, INFN Lattice QCD QED corrections to meson decay rates in
25.300.000
Constantia Alexandrou, Cyprus University Nucleon structure using lattice QCD simulations with physical pion mass
46.800.000
Yanick Sarazin, Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA) GYSELA-ROTATION
34.000.000
Massimo D'Elia, Pisa University Strong interactions in strong magnetic fields
10.000.000
Santiago Badia, CIMNE (Universitat Politecnica de Catalunya) Extreme scale domain decomposition solvers for computational mechanics
21.000.000
Mattia Falconi, Tor Vergata Univ. Design of self-assembling DNA nano-cages provided with pH and temperature controlled gates for the target-delivery of biomolecules
29.000.000
Gianluigi Bodo, INAF From local to global models of accretion discs: beyond the alpha prescription


ISCRA
Ministero dell'Istruzione dell'Università e della Ricerca
Astrophysics and Plasma Physics
1.000.000
Dario Borgogno, PoliTO
Analysis of kinetic effects in collisionless plasmas through the FLR-Landau fluid model
990.000
Andrea Mignone, Torino
Pressure-balanced and force-free magnetized jets
900.000
Salvatore Orlando, INAF
The remnant of SN 1987A: a Roseta stone for core-collapse supernovae
1.400.000
Fabio Reale, Palermo University
The bright life of entwined magnetic tubes
1.000.000
Stefano Sinigardi, Bologna University, Physics Department
PIC simulations for X-ray production
Computational Chemistry
776.602
Giovanni Barcaro, Istituto per i Processi Chimico-Fisici UOS Pisa
Ultra-thinternary metal oxides: structure and electronic properties
600.000
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Turbulence dynamics in the separation region of wall bounded flows
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Conor Hogan, CNR-ISM and ETSF
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1.560.000
Ivan Marri, Modena and Reggio Emilia University, Dept. of Science and Methods for Engineering
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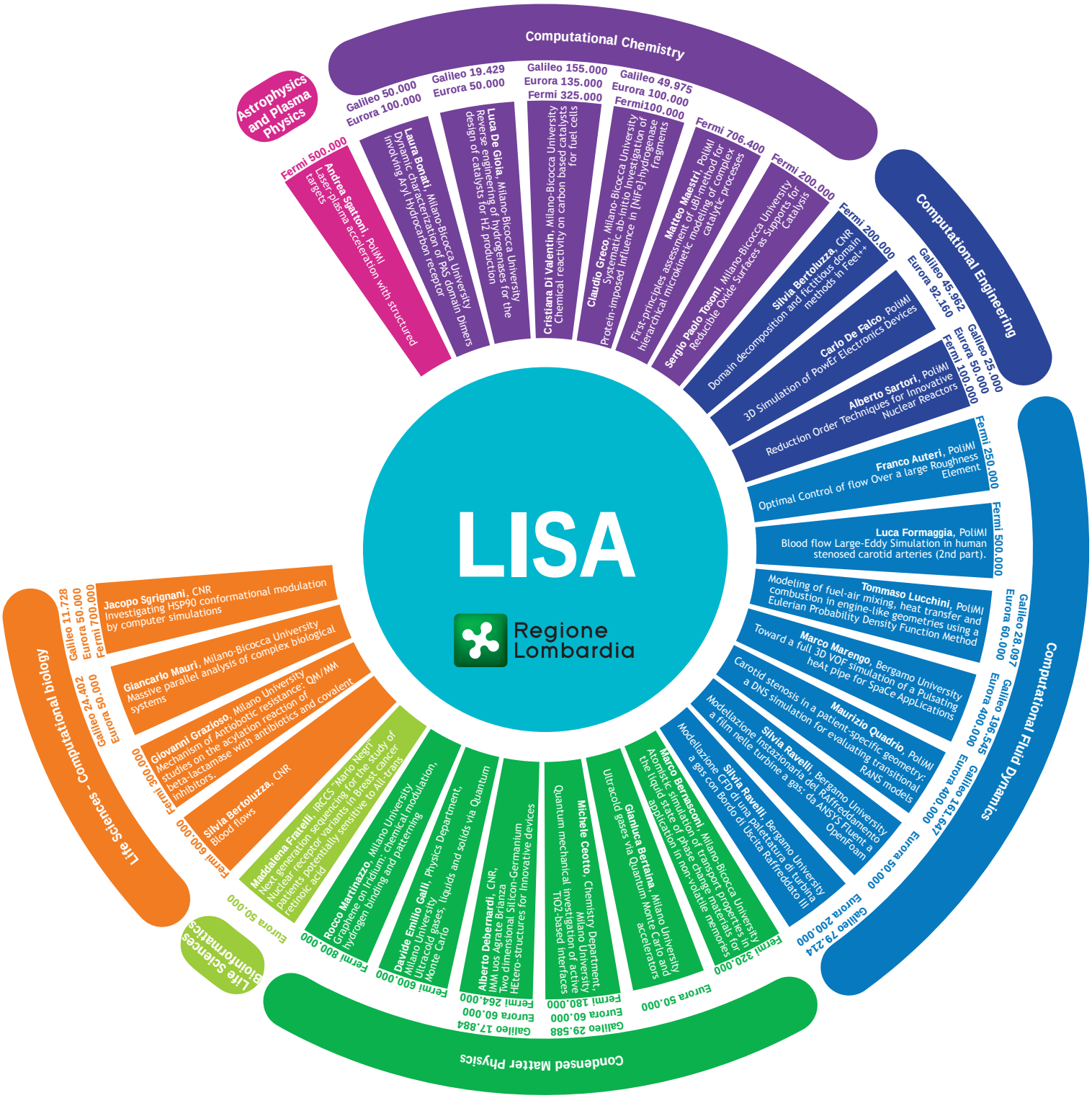
LISA
Regione Lombardia
Computational Chemistry
Astrophysics and Plasma Physics
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Computational Fluid Dynamics
Life Sciences - Computational biology
Life Sciences Bioinformatics
Condensed Matter Physics
Andrea Sgattoni, PoliMI
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Convective models of accretion discs

Accretion is the process through which matter gradually falls on a central object, releasing its gravitational energy and generating heat and radiation that we can observe. Accretion typically occurs by forming a disc structure and accretion discs are ubiquitous in the universe: they can be found in the nuclei of galaxies, around supermassive black holes, and around stars both at the beginning and at the end of their life. They can power some of the most energetic phenomena in the universe and understanding how they work is very important for the comprehension of different astrophysical problems like how stars are formed or what happens in the central cores of galaxies. The matter in the disc orbits around the central object like a planet around the Sun and it would continue forever if it there didn't exist a way to extract its angular momentum. An efficient transport of angular momentum can occur only if the disc is turbulent. For determining the structure of an accretion disc one has therefore to answer to a series of complex physical questions: How turbulence develops and what are its properties? How the turbulence regenerates the magnetic field by dynamo action? How the energy dissipated by turbulence is transported to the surface layers of the disc to give origin to the observed radiation? The analysis of these complex processes can be done only through three-dimensional magnetohydrodynamic simulations on the most powerful supercomputers.

Recently, by simulating in detail a small portion of a disc, we discovered that there are situations in which the transport of the heat generated in the central layers to the disc surface is accomplished by convection and, in this case, the process of angular momentum transport is very much enhanced. When convection sets in, the disc becomes then more luminous. This process can be at the base of some of the variability behaviors observed in many astrophysical objects. Our project aimed at studying in more detail the properties of these convective discs and to determine where, in an accretion disc, convective regions can be found. The simulation project was enabled through the Partnership for Advanced Computing in Europe (PRACE) on HPC system Fermi at Cineca. The simulations were performed with the PLUTO code, developed by our group, with computational boxes of up to 15,000,000 grid cells, on up to 32,000 cores. We were able to build more realistic local models in which convection occurs only in the central layers and, in addition, by patching together such local models we were able to obtain the global structure of an accretion disc. In this way we showed that in every disc one can find a region in which convection must play a fundamental role.

Gianluigi Bodo, Paola Rossi
INAF Torino Astrophysical Observatory

Andrea Mignone
Torino University

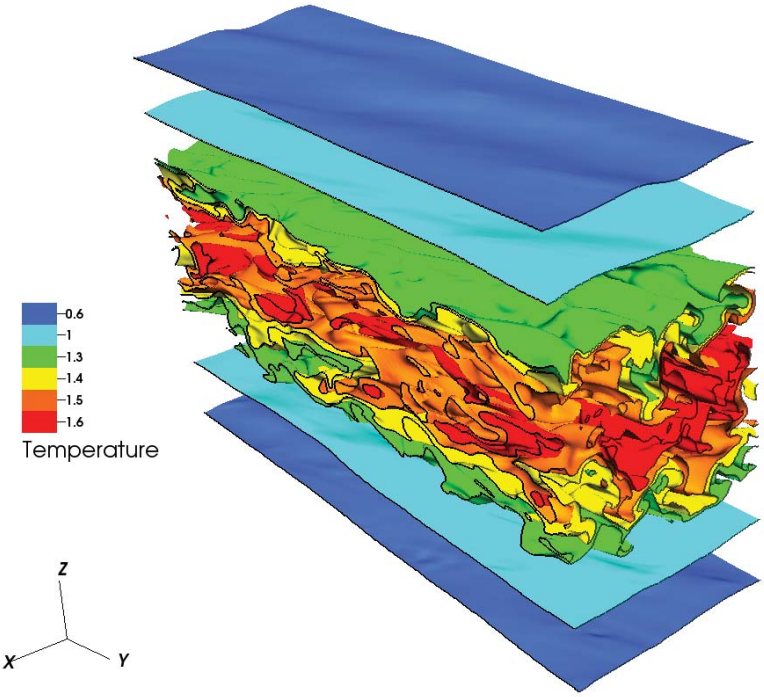
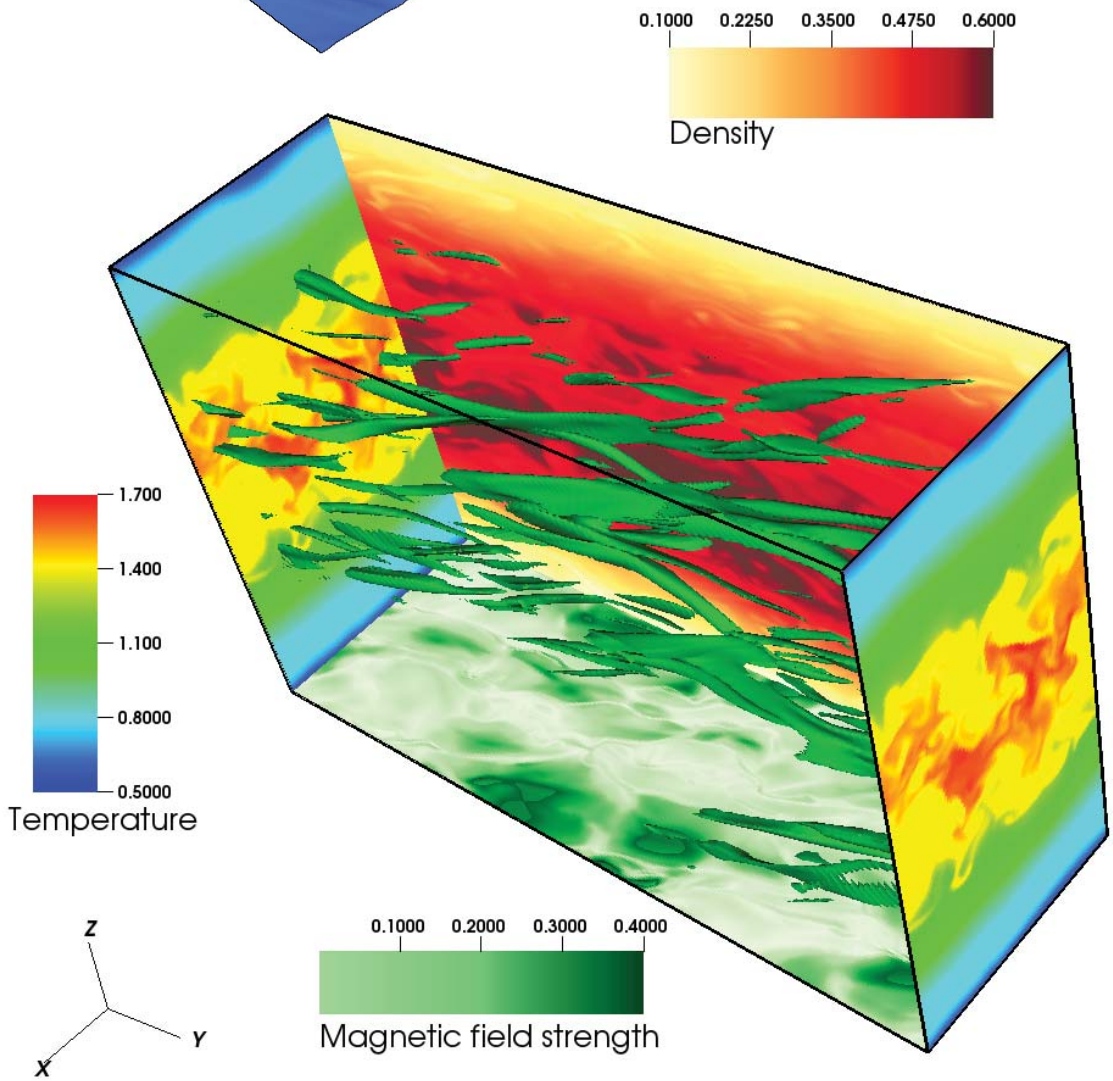


Figure 1: The figure shows equicontour surfaces of the temperature distribution, for a simulation in which heat is transported by convection in the central layers and by radiation in the surface layers. The contour surfaces in the center are distorted by convective motions, while in the surface layers equicontour surfaces become almost planar.

Figure 2: The figure shows equicontour surfaces of the magnetic field strength. We observe the formation of elongated structure in the direction of the flow (azimuthal direction). We also show the temperature distribution on the two lateral sides of the box, the density distribution on the back face of the box and the magnetic field strength on the bottom face. Temperature and density distributions show the presence of convective cells in the central part of the box.



Simulating the forces between quarks in the presence of exceptional magnetic backgrounds

Strong interactions are described by Quantum Chromodynamics (QCD), the theory of quarks and gluons. One distinctive feature of QCD is the emergence of a linearly rising potential between quarks, proportional to a force of around 10 tons, usually called string tension. This is a typical non-perturbative property of QCD, which can be explored by numerical simulations of the theory (Lattice QCD).

Quarks are also subject to electroweak interactions, which in general induce small corrections to QCD dynamics. The situation can be different in the presence of exceptional electromagnetic backgrounds, strong enough to directly affect the QCD scale. Such huge magnetic fields are expected in non-central heavy ion collisions and may have been produced at the cosmological electroweak phase transition, with magnetic fields in the range 10^{15} - 10^{16} Tesla.

One of the purpose of this project has been to explore the effect of the magnetic field on the string tension between quark-antiquark pairs, which a previous exploratory study [1] has shown to become anisotropic, with the force being stronger/weaker in the directions orthogonal/parallel to the magnetic field. By means of state-of-the-art numerical simulations, exploiting physical quark masses and lattice spacings below 0.1 fermi, we have been able to confirm such phenomenon, extrapolating results to the continuum limit and also resolving the angular dependence of the quark-antiquark potential. This has been possible thanks to the resources provided on Fermi. Results are especially relevant to the physics of heavy quark bound states [2].

Massimo D'Elia
Pisa University

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Phys. Rev. D 89, no. 11, 114502 (2014) [arXiv:1403.6094 [hep-lat]].
[2] C. Bonati, M. D'Elia and A. Rucci,
"Heavy quarkonia in strong magnetic fields"
Phys. Rev. D 92, no. 5, 054014 (2015) [arXiv:1506.07890 [hep-ph]].

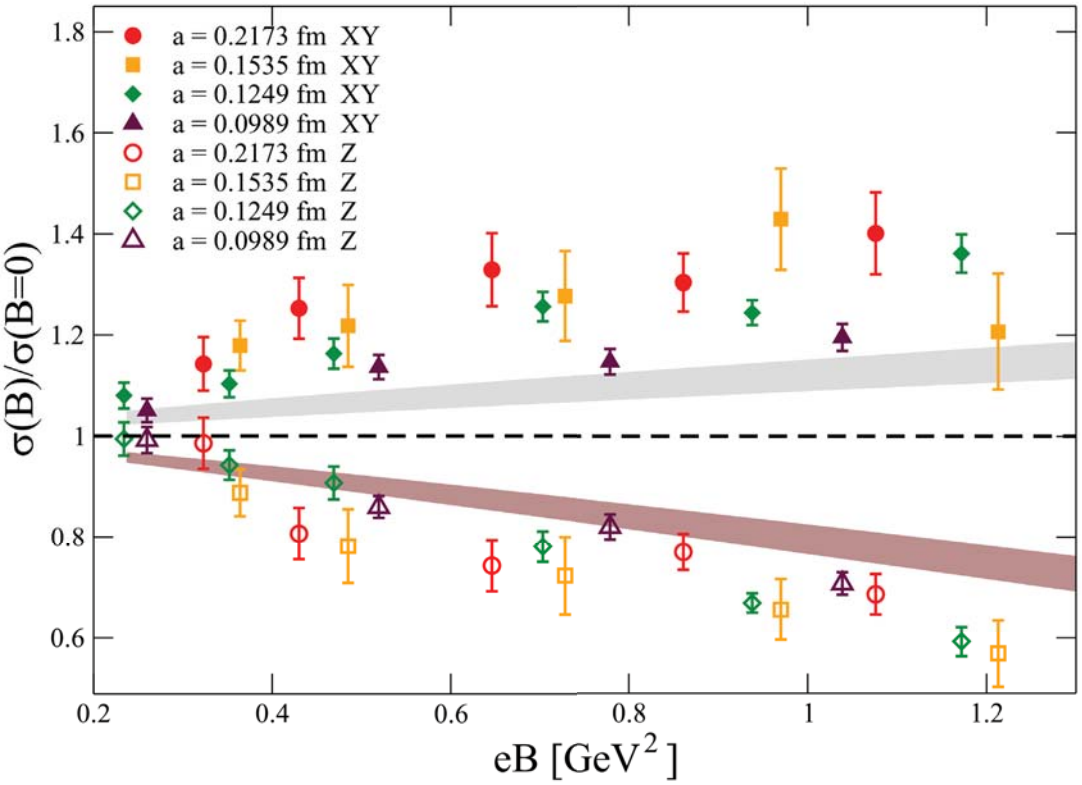


Figure 1: String tension as a function of the magnetic field (directed along the z axis) along different directions and for different lattice spacings. The colored bands represent continuum extrapolated results.

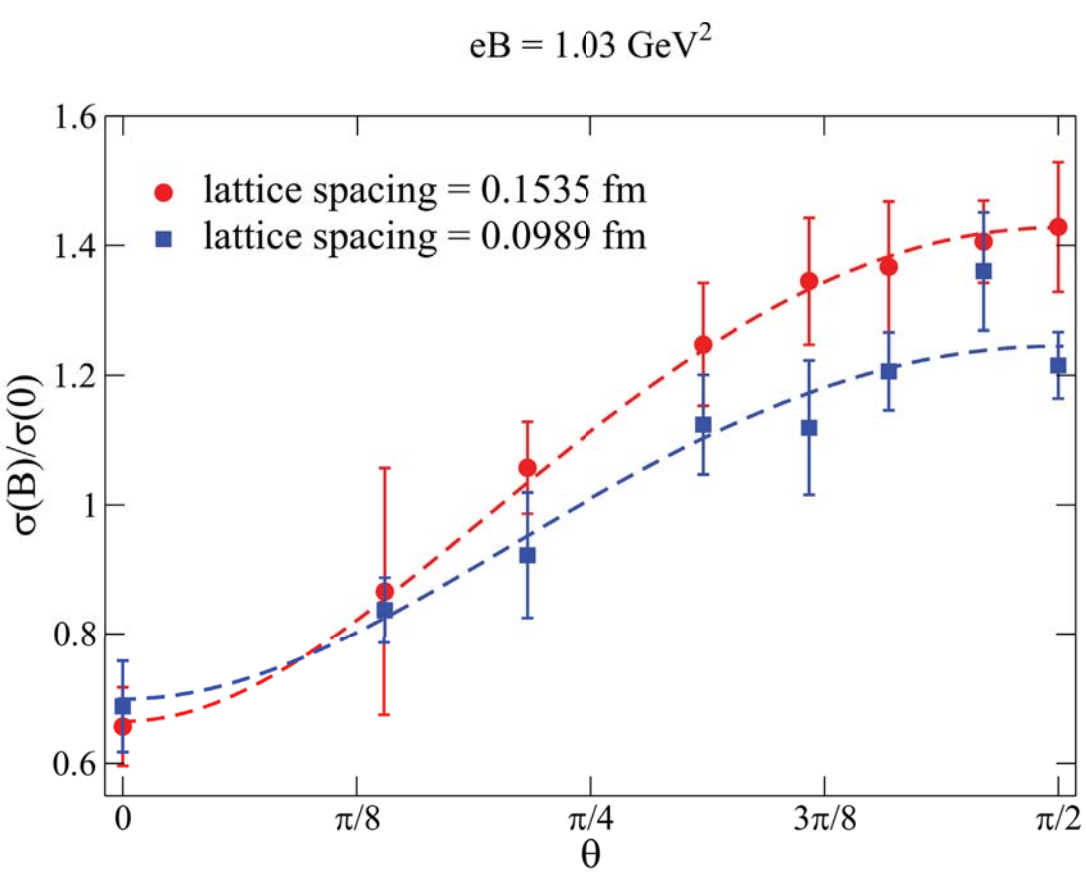


Figure 2: Dependence of the string tension on the angle between the magnetic field and the quark-antiquark pair. Results are reported for two different lattice spacings.

Direct Numerical Simulation of oscillatory flow over a rough bottom composed of fixed and movable particles

Many problems of coastal engineering, such as coastal erosion, stability of marine structures, the planning of dredging activities etc., are strongly affected by a reliable and accurate evaluation of sediment transport. However, the available models for quantifying the sediment transport rate are largely based on empiricism and in many cases they provide poor predictions. The project is devoted to the investigation of a few key issues, relevant for the evaluation of the sediment transport rate under sea waves.

In the first part of the project, we investigated the influence of the bottom roughness on the flow field generated by an oscillating pressure gradient close to a plane bottom for moderate values of the Reynolds number. The wall roughness was made with spheres arranged in a regular pattern. Computational resources were granted on Fermi in the context of a PRACE project. A preliminary exploration of the parameter space (Mazzuoli & Vittori, submitted) showed that turbulent vortices forming over the rough wall are strongly influenced by the roughness size.

Indeed, depending on the value of the Reynolds number and on the size of roughness elements, three flow regimes were identified which are briefly described in the following. The laminar regime is characterized by negligible fluctuations over the average flow field. By increasing the Reynolds number, for spheres of diameter comparable with the thickness of the Stokes layer, the transition to turbulence results from an instability process promoted by the adverse pressure gradient (similarly to the smooth wall case). Finally, by increasing the size of the spheres, the hydrodynamically rough regime is attained, where turbulence originates from the interaction of the wakes behind the roughness elements and significant values of the turbulent kinetic energy are present throughout the wave cycle.

Then, one of the recent experiments of Carstensen et al., Phys. of Fluids (2012) where the formation of turbulent spots was observed over a plane bottom with wall-fixed sand, was reproduced. The size of the computational domain was the same as the measurement section of the experimental facility, requiring a remarkable computational effort ($\mathcal{O}(10^{10})$ grid points). Turbulent spots and coherent vortex structures are particularly relevant to sediment dynamics, since they cause large values of the shear stress concentrated in small regions close to the bottom, which in turn cause sediment movement and sediment resuspension. In the present investigation no turbulent spots were observed. Only in one of the simulations, the transition to turbulence occurred for the same Reynolds number as in the experiment and for a diameter of the spheres two times larger than the average size of the sand grains. Indeed, during the deceleration phase of the fifth wave half-cycle, the flow experienced the natural transition when hairpin vortices and turbulent structures formed (see Figure 1). The formation of turbulent spots was finally observed during the seventh wave half-cycle.

The second part of the project investigated the dynamics of sediment particles dragged by the oscillatory flow. DNS were used to determine the flow field. The flow was fully resolved also in the vicinity of the individual particles (Uhlmann, J. of Comp. Phys., 2005), approximated by rigid heavy spheres, while the influence of the particle motion on the fluid flow was explicitly taken into account. Particle collisions were simulated by a soft collision model (Discrete Element Method). A preliminary investigation (Mazzuoli et al., submitted) was aimed at validating the model of sediment dynamics. The experiment by Hwang et al., Proc. 8th Int. Conf. Hydrodynamics (2008), who observed that spheres, initially aligned on a flat wall in the direction of propagation of surface waves, in few oscillating cycles lose their alignment and form transversal chains, was reproduced (see e.g. Figure 2). Then, the evolution of a movable bed composed of ~ 15 layers of movable spheres ($\mathcal{O}(2 \times 10^5)$ particles), exposed to an oscillatory flow, was simulated. After few oscillating periods, the early stages of the formation of two-dimensional bedforms were observed (see Figure 3).

G. Vittori, M. Mazzuoli
Department of Civil, Chemical and Environmental Engineering (DICCA), University of Genoa, Italy

M. Uhlmann, A. Kidanemariam
Institute for Hydromechanics (IfH), Karlsruhe Institute of Technology (KIT), Germany

Acknowledgments
We acknowledge the PRACE 7th award and Cineca, for the availability of high performance computing resources and support.

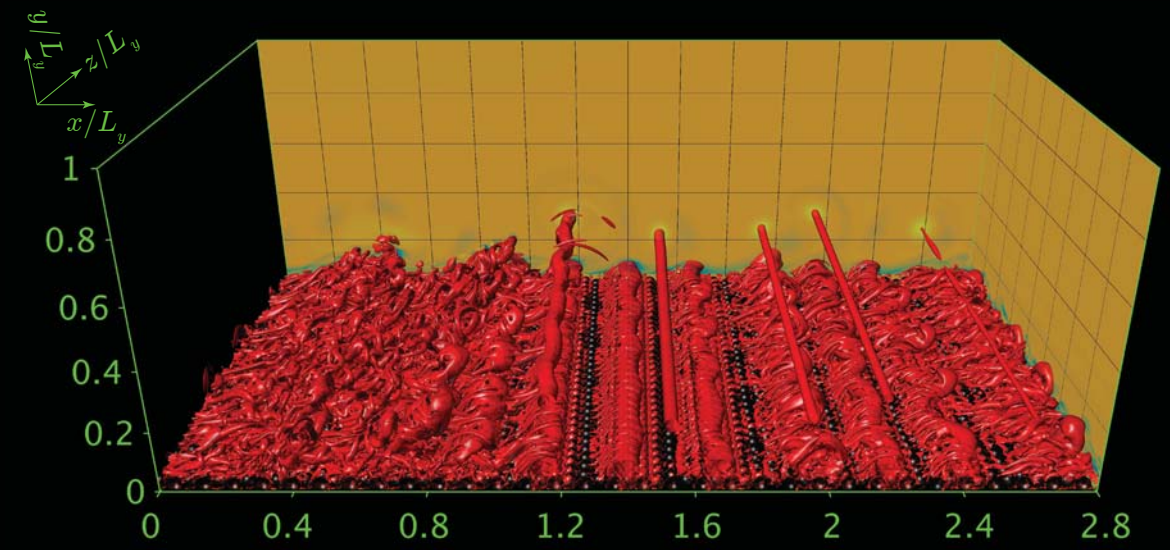


Figure 1: Vortices forming during the transition to turbulence (deceleration phase of the wave cycle) and visualized with the λ_2 criterion (red isocontours). Lateral faces of the computational box are coloured by the spanwise vorticity. Axis are scaled by $L_y = 51{,}24\delta$, where δ denotes the thickness of the Stokes layer. Flow is directed rightward.

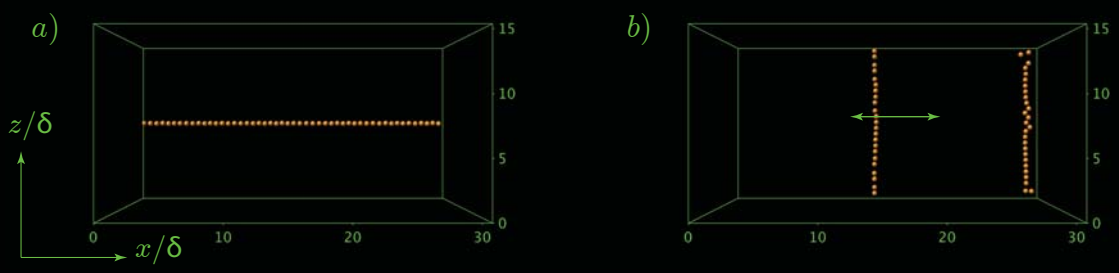


Figure 2: Top view of the particle arrangement. Flow oscillations redistribute the spheres from their initial streamwise-aligned position (a) into spanwise-oriented chains (b) after $\mathcal{O}(10)$ oscillation periods. Axis scaled by the thickness of the Stokes layer, δ.

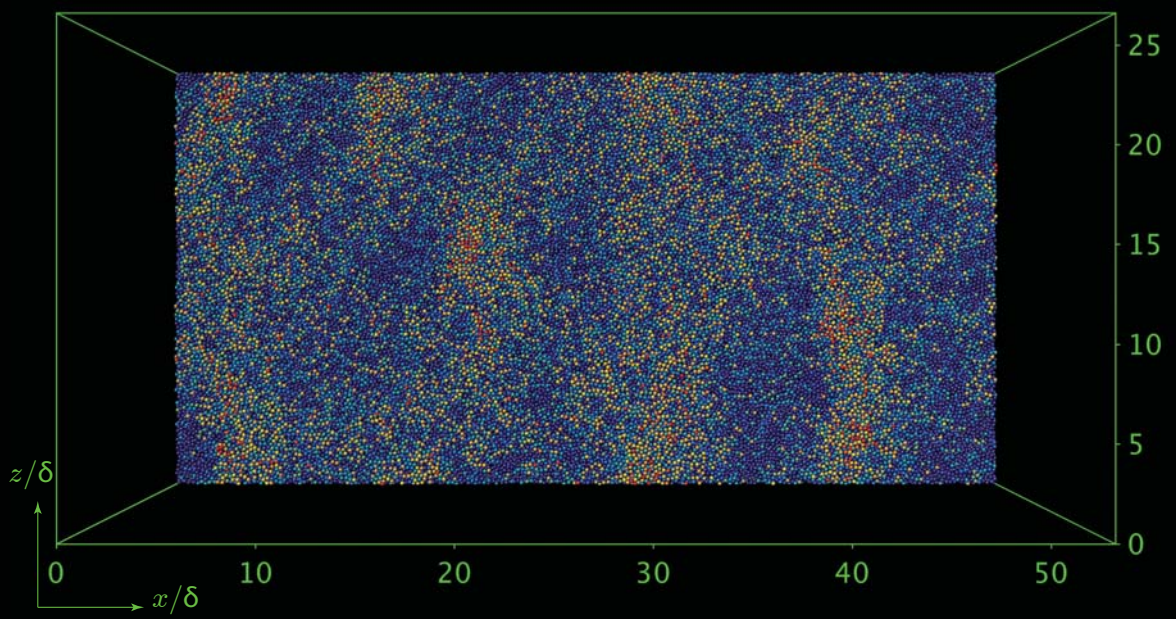


Figure 3: Top view of sedimentary patterns forming on the movable bed at the top of the acceleration phase of the 10th oscillation period, when the flow is directed leftward. Spheres are coloured by their distance from the bottom. Axis are scaled by the thickness of the Stokes layer, δ.

Effect of the stirrer orientation and positioning on the reverberation chamber statistics

Our in-house parallel finite-difference time-domain (FDTD) code was used to simulate the influence of the orientation and positioning of the stirrer on the reverberation chambers statistics. The code includes a full-wave electromagnetic solver based on the FDTD method, a fast Fourier transform (FFT) module (based on FFTW library) to obtain the frequency domain behavior, and a statistical module. It implements a hybrid parallelization using MPI and OpenMP protocols. A more complete description of the code can be found in the "2014 Cineca HPC Report".

This work analyzes how the position of the stirrer rotation axis influences the field uniformity, the number of independent positions, the Rician K-factor, and the Anderson-Darling goodness-of-fit test. Initially, the rotation axis was moved parallel to the z-axis from a corner to the center of the reverberation chamber in fifteen positions. Then, the rotation axis was rotated to be parallel to both the x- and the y-axis, and twelve different scenarios were analyzed, using the same stirrer height and enlarging the gap between the paddles to fit the chamber side. All the other parameters like stirrer shape, antenna positions and the working volume remained the same. We analyzed a stirrer that consists of three blades at some spatial positions, while the paddles are only 0.15 m from the reverberation chamber walls. Several factors contribute to enhance the stirring performance, such as the chamber volume related to the operating frequency, and the chamber loading condition. The shape of the rotating paddles is also an important parameter: in particular, its dimension plays a fundamental role in the stirring efficiency. A significant stirrer performance enhancement occurs when the blade width is increased.

The simulation for all the angles when the stirrer rotates along an axis requires one hour time, while an equivalent experimental measurement is much more expensive and time consuming. In particular, to move and turn the rotation axis with both the paddles and the motor makes it a challenging measurement, and it can greatly increase the time required.

Simulations show that the position and the orientation of the stirrer rotation axis has only a weak influence on the reverberation chamber performance. Consequently, in the design stage of a reverberation chamber it is better to give priority to other parameters, the reverberation chamber designer can then choose the rotation axis of the stirrer free from electromagnetic constrains, while taking into account the mechanical requirements, as well as the optimization of the working volume. Simulations are useful for designing the best shape of the stirrer to improve the reverberation chamber performance.

The availability of a reliable and optimized FDTD code for reverberation chamber simulations, along with a high performance computer, allows us to easily investigate the stirrer performance in a reverberation chamber.

Luca Bastianelli, Valter Mariani Primiani, Franco Moglie
DII, Marche Polytechnic University

Gabriele Gradoni
School of Mathematical Sciences, University of Nottingham, United Kingdom

Acknowledgments
We acknowledge PRACE for awarding us access to resource FERMI based in Italy at Cineca.

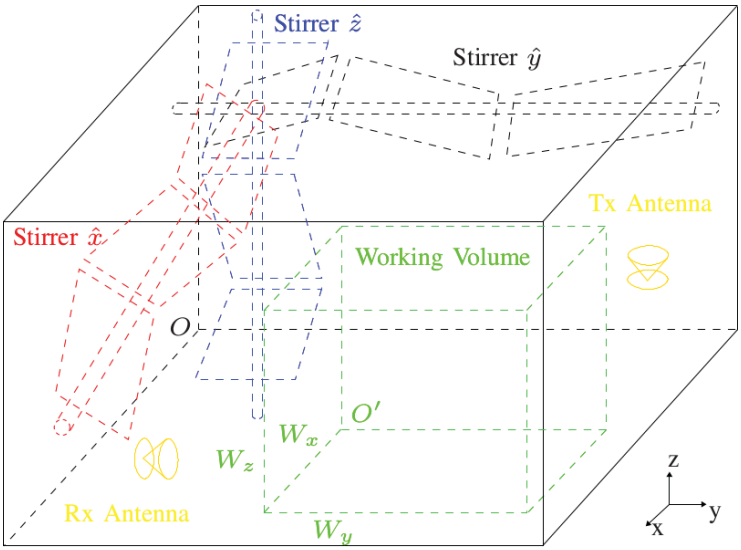


Figure 1: View of the simulated reverberation chamber with the stirrer parallel to each Cartesian axis.

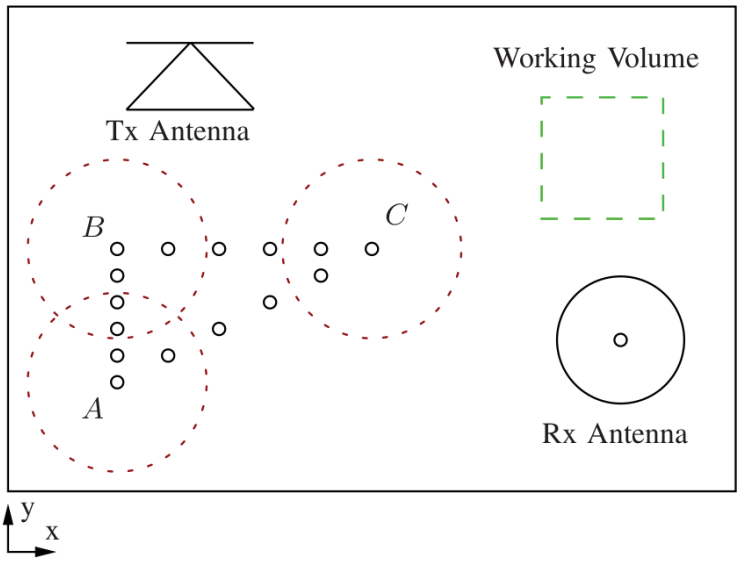
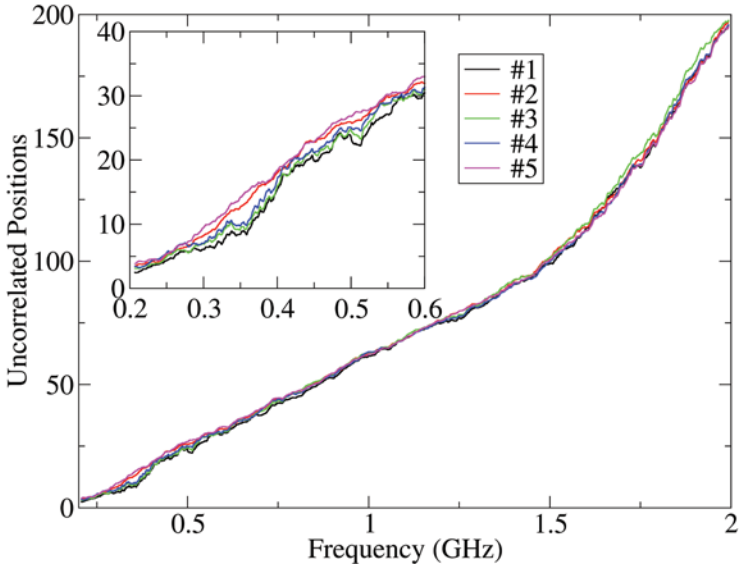
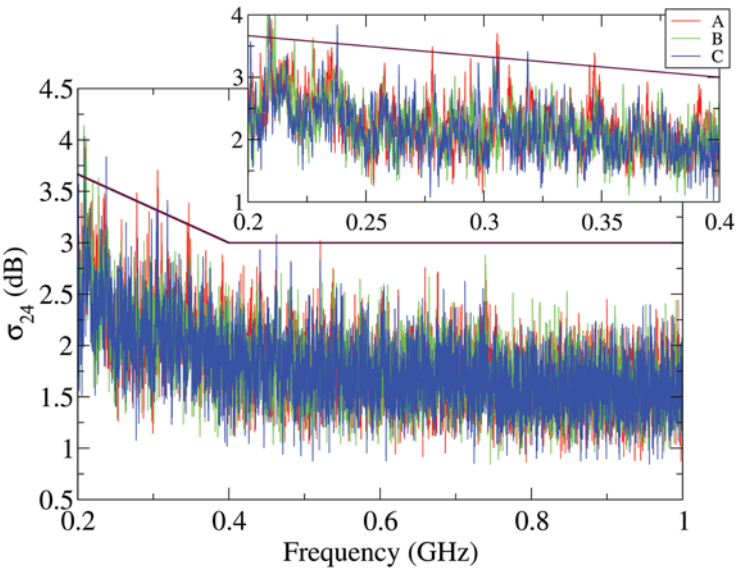


Figure 2: Reverberation chamber, with transmitting and receiving antennas, investigated working volume, and the positions of rotation axis of the stirrer.

Figure 3: Simulated number of uncorrelated positions, changing the direction of stirrer axis (#1, #2, #3) and increasing the gap between the paddles (#4, #5).

Figure 4: Simulated standard deviation of the field uniformity for three different center of the rotation axis parallel to the z-axis.





Solving the full vectorial Maxwell equation with a parallel algorithm for the determination of the opto-mechanical forces in 3D random media

In the field of optomechanics, the benefits of randomness have not yet been investigated, even if, from the perspective of optically activated nano-structured devices, understanding opto-mechanical forces (OMFs) due to the multiple scattering and localization phenomena of light is pivotal.

Simulations have been carried out by means a parallel code based on a finite-difference-time-domain algorithm to solve the fully vectorial Maxwell equations within 3D random systems. Because of the small values of the OMFs, we consider the light propagation within few-microns-sized systems made of disordered assemblies of dielectric nano-particles. The code allows to combining the calculus of the OMFs and the analysis of the light transport regime of ultra-short light pulses. We find that with increasing disorder the transverse components of the OMFs statistically broaden, correspondingly the diffusion constant and the transport mean free path decrease, and the optical pressure reaches a maximum. This maximum shows that the momentum transferred to a disordered micron-sized composite object increases when approaching the localization regime. Our results foster the exploitation of photon random walk in light-induced pressure based micro-devices.

We performed disorder average over tens of different disorder configuration. Typical computation required about 4096 cores for the computation of about 1 hour in real time on the IBM Blue Gene/Q Fermi machine in the framework of the ISCRA-HPC project Tracton-HP10BEMXCX entitled “Ab initio simulation on tractor light beams due to the optical nonlinear response”.

Silvia Gentilini, Claudio Conti
CNR-ISC

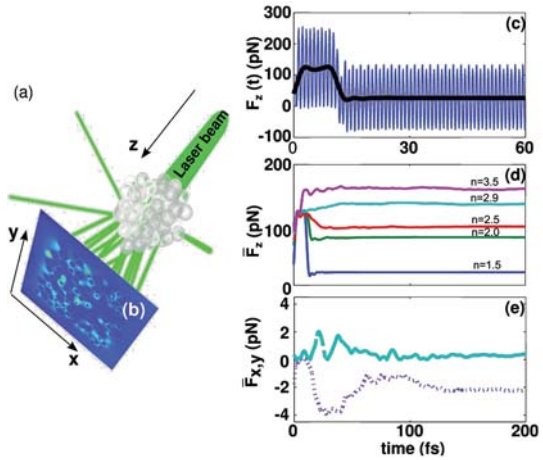


Figure 1:
(a) Sketch of the physical system considered in the 3D-FDTD numerical simulations; (b) intensity spatial distribution of the output electric field; (c) time dynamics of the OMF z-component, $F_z(t)$: the fast oscillations are due to the optical carrier period of the light source; the superimposed thick curve is obtained by spectral filtering the fast oscillations; (d) time-dynamics of disorder averaged $F_z(t)$ for different particles refractive index n and fixed system length L = 2.0μm; (e) as in (d) for the transverse components $F_x(t)$ (dotted line) and $F_y(t)$ (continuous line) for n= 2.5 particles refractive index.

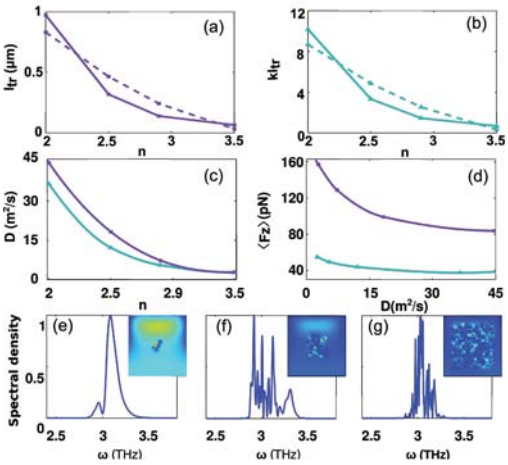


Figure 2:
(a) Photon transport mean free path ℓ_{tr} versus n for the system sizes L= 1.0μm (continuous line) and 2μm (dashed line). (b) Product $k\ell_{tr}$ versus n obtained from the panel (a) for the system size L= 1μm (continuous line) and L=2μm (dashed line). (c) Diffusion coefficient D vs n obtained for the system sizes L= 1.0μm (■) and 2.0μm (▲). (d) Stationary value of the $\langle F_z \rangle$ vs diffusion coefficient D for L= 1.0 (■) and 2.0 μm (▲) system sizes. (e-g) Spectral content of the output electric field for the highest particles refractive index (n = 3.5) and different system sizes L= 0.5 (e), 1.0 (f) and 2.0μm (g). The insets show the intensity spatial distributions of the output electric fields in the (x, y) plane at z = L.

Turbulence dynamics in the separation region of channels with lower curved walls

Wall bounded turbulent flows and boundary layer separation represent challenging subjects in fluid dynamics since, for example, the largest part of the energy spent to move vehicles through fluids is dissipated in the boundary layer close to the walls and/or in the turbulent wake behind the vehicle.
The fluid streaming around bodies cannot follow the actual body shape and becomes detached due to viscous effects. This causes the flow to separate, i.e. the fluid closest to the body boundary starts flowing in a reverse direction, giving rise to intense turbulent fluctuations, recirculating regions and wakes.
This research addresses wall bounded separated flows to understand and characterise the turbulence dynamics in the presence of strong non-homogeneous effects. To fill the gap between idealised conditions, such as plane channel flows, and actual flow geometries where the wall curvature
generates a massive separation, we consider a channel with a lower curved wall. The Direct Numerical Simulation (DNS) approach is exploited to tackle the turbulence conundrum in such highly non-homogeneous conditions at a relatively high Reynolds number. The DNS were carried out using resources granted by the projects Iscra-C #HP10CFDV6L, Iscra-B #HP10BII83O and PRACE #2014112647, which allowed the use of the computing capabilities of the Tier-0 machine Fermi at Cineca. State of the art simulations were carried out at a Reynolds number of 10:000 that is the highest currently explored in such geometry. A typical outcome of the simulations is presented in Figure 1 which shows a stream-wise 2D plane highlighting the massive flow separation behind the bump. Figure 2 shows the ensuing vortical structures which feed turbulent fluctuations in the wake behind the bump.

J-P. Mollicone, F. Battista, P. Gualtieri, C.M. Casciola
La Sapienza Roma University,
Department of mechanical and aerospace engineering

Figure 1: Snapshot of the instantaneous stream-wise velocity intensity in x-y plane at Re = 10:000. The flow is from left to right, with a separated region behind the bump and the thin shear layer generated at the tip of the bump.

Figure 2: 3D view of the coherent vortical structures generated by the flow separation just behind the bump denoting the highly intense turbulence activity at small scales.

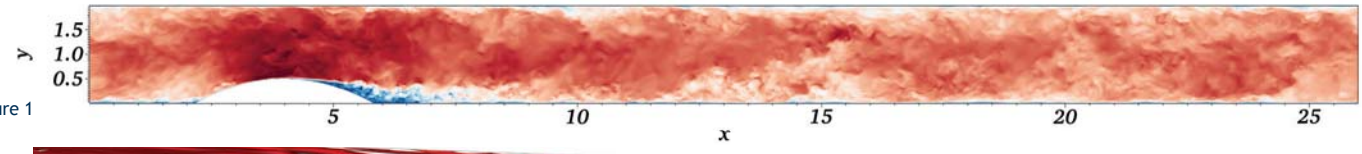


Figure 1

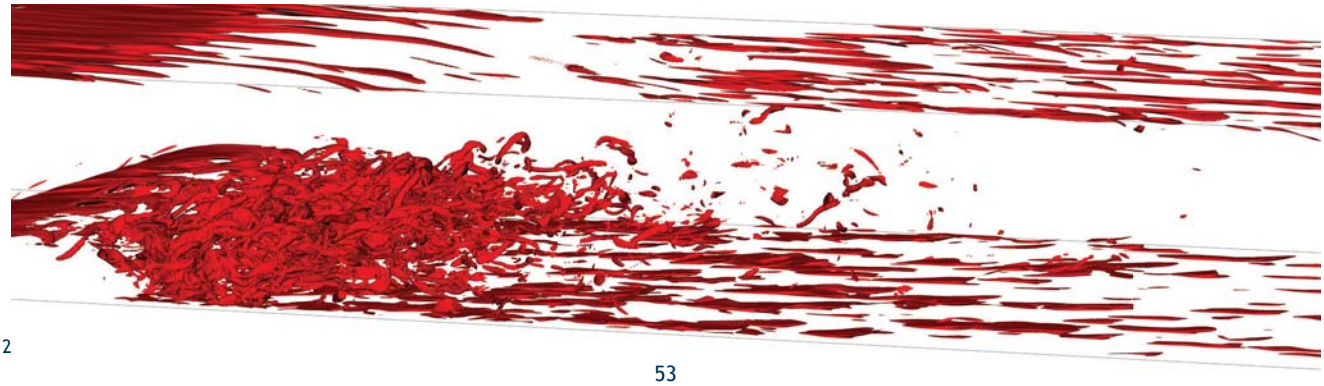


Figure 2

Enhanced VOF Simulations of Two-Phase Flows With Phase Change

Anastasios Georgoulas
Marco Marengo
University of Bergamo, Department of Engineering and Applied Sciences

The present work deals with the development, validation and application of an enhanced Volume Of Fluid (VOF) method for the simulation of boiling heat transfer phenomena that occur within confined channels. The overall development of the model, has been conducted within the OpenFOAM CFD ToolBox. In more detail the already implemented VOF solver of OpenFOAM has been further improved in order to dampen out the development of parasitic/spurious currents at the two-phase flow interface. Moreover, heat transfer and phase-change have been added to the solver in order to render it capable of simulating boiling heat transfer phenomena. Some examples of the validation of the solver against experimental results and analytical solutions are illustrated in Figure 1. In Figure 2, indicative results from the application of the validated solver for the case of flow boiling within confined channels, are shown. The ultimate goal of the proposed work is to develop a "Direct Numerical Simulation" tool that can be applied for the simulation of two-phase flow and heat transfer phenomena that take place within two-phase flow cooling systems such as heat pipes and pulsating heat pipes. More details regarding the overall achievement in the proposed direction can be found in recent works by the Authors [1]-[4].

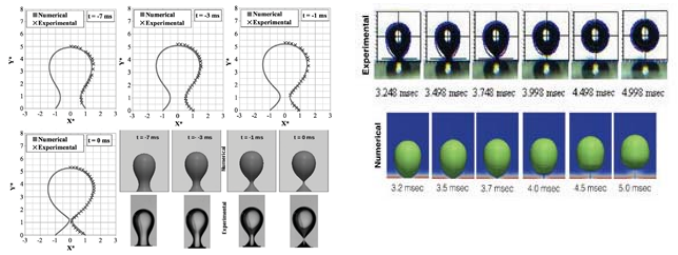


Figure 1

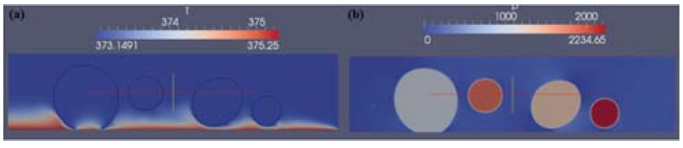


Figure 3

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Figure 1: Comparison of numerical with experimental results: quasi-static bubble growth and detachment from submerged orifices in isothermal liquid pools [2] (top), evaporative bubble growth and detachment from superheated plates [3] (bottom).

Figure 2: Numerical simulation of flow boiling of water in a micro-channel [4].

Figure 3: Final temperature (a) and relative pressure (b) distribution, at a central vertical section within the computational domain at the last time instance of Figure 2 [4].

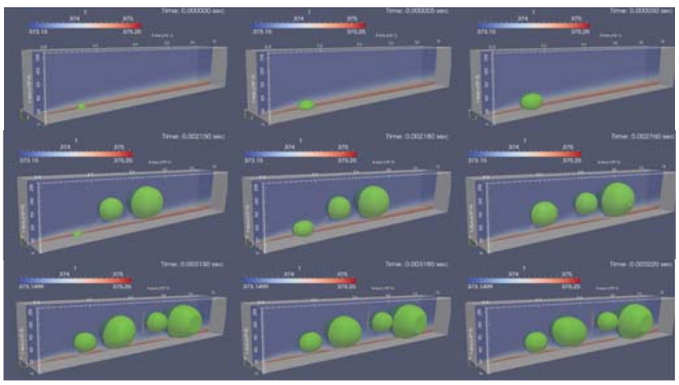

Figure 2

Electronic Coupling Effects in Silicon Nanocrystals: Ab-Initio Results

Arrays of closely packed nanocrystals (NCs) show interesting properties that can be exploited to maximize solar cells performances. Recently, experimental and theoretical works [1-2] have proven that NCs interplay can induce new energy and charge transfer carrier multiplication (CM) effects, termed Space Separated Quantum Cutting (SSQC) and Coulomb Driven Charge Transfer (CDCT), respectively. These effects, that can be exploited to increase solar cell photocurrent, have been quantified for the first time by our group through first principles simulations. By considering systems of coupled Si-NCs and thank to the
numerical resources offered by Cineca, we have proven that:
1) the delocalization of the wavefunction boosts the relevance of both SSQC and CDCT effects.
2) NCs interplay can lead to a reduction of the energy gap of the system. This effect depends on the NC-NC separation, on the NCs orientation and on the NCs surface properties [4].

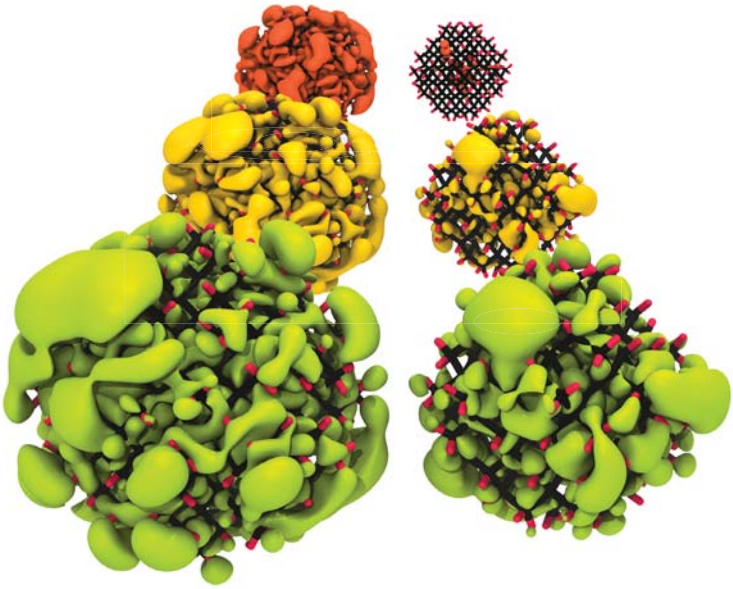

Figure 1: When NCs are placed in close proximity, wavefunctions delocalize over the entire system. In these conditions, both SSQC and CDCT rates are maximized.

3) SSQC and CDCT occur in an asymmetric way, more likely from the smaller to the largest NC. This effect leads to an intensification of the photoluminescence (PL) activity in the larger NC, and therefore to a red shift of the PL peak.
4) SSQC rates depend on the selected decay path and can not be estimated using the dipole-dipole approximation. A detailed estimation of CM energy transfer processes generated from delocalized states requires an accurate evaluation of the screened Coulomb matrix elements without assuming a simplified form of the Coulomb interaction [4].

I. Marri, S. Ossicini
University of Modena and Reggio Emilia,
Department of Science and Methods for Engineering

M. Govoni
Institute for Molecular Engineering, the University of Chicago

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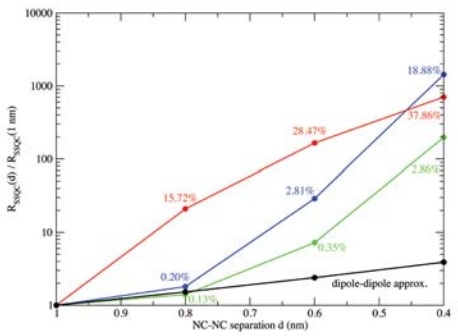

Figure 2: Increment of SSQC rates are calculated by selecting three different decay paths ignited by states with different energies (green, red and blu lines). For all the considered NC-NC separation we report the localization of the state on the smaller NC. Results are compared with the ones obtained using the dipole-dipole approximation (black line).

MHD modeling of a coronal downflow

The corona is the outer region of solar atmosphere. It is composed by ionized gas at a temperature greater than 1 million degree, called plasma. It is composed by a multitude of closed magnetic structures. The interaction with the underlying atmosphere, the photosphere, can lead to the break of this structures. When this happens, great amount of plasma can be ejected from the surface into the outer atmosphere. Depending on the ejection speed, the plasma can fall back to the surface or it can leave the Sun. The former case is of great interest in astrophysics because it is a template of a more general issue: the accretion in young stars.

The observations of the Sun in the Extreme Ultraviolet band show that, when dark downfalling plasma is channeled by the magnetic field, the channel brightens and the obvious question is why and how.

The IscraC project 'MHD modeling of a coronal downflow' studied the interaction of downfalling blobs of plasma with a strongly magnetised atmosphere, with the aim to explain the origin of the observed emission.

We build a 3D MHD model of the solar atmosphere with gravity, thermal conduction, radiative losses, immersed in a closed magnetic field. The computational box is 33 million cells and we used the 3D-MHD PLUTO code to run the simulations on 4096 Cineca/Fermi cores in about 2 milion of CPU hours.

This work has been presented in international meetings:

- '2nd Meeting SolarNet' (2-5 February 2015,Palermo);
- '7th Coronal Loop Workshop' (21-23 July 2015, Cambridge UK).

Antonino Petralia
Palermo University

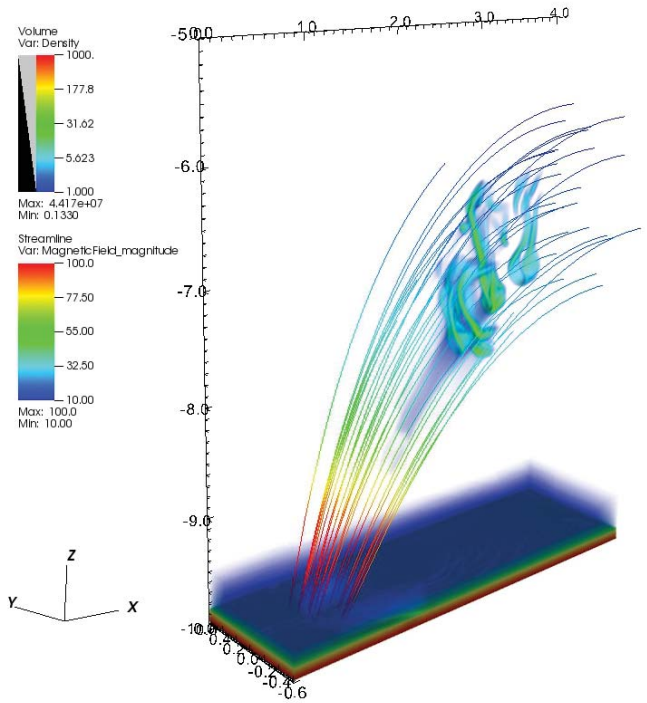

Image of the plasma density and Magnetic field lines after 100 seconds of evolution of the downfalling blobs.

Controlling the screw-sense in switchable self-assembling polymers

Understanding the switching and self-assembly of macromolecules into predictable patterns on surfaces is noteworthy for the bottom-up design of functional nanostructures [1,2]. Artificial polymers can indeed exhibit a switchable screw-sense whose inversion is conducted by chemical or photo stimuli [3-4].

In these regards, the chiral switch properties of polyfluorene-based polymers (poly(9,9-dioctylfluoren-2,7-diyl) (PDOF)) have been elucidated through enhanced sampling free-energy simulations [5]. Those indicate that the chirality induction is feasible through a stepwise switching of the fluorene-fluorene dihedrals. The chiral switch occurs only when the polymer is deposited on a support and not on an isolated chain or aggregated phases of the polymer (Figure a)-d)), indicating that the solid surface may facilitate the achiral-to-chiral transition as an inert supramolecular scaffold.

The accuracy of the proposed chiral switching mechanism was assessed by calculating the electronic UV spectra of 2,2'-difluorenyl as a dimer model at the TDDFT level through the B97-D functional[6] (Figure e). This model is considered reasonable as it may represent the shortest chiral sequence in PDOF.

Experimental UV spectra [7] indicated overall blue-shifts and hypochromism (Figure f). Intensities of the lower-energy bands at 430 nm and at 400 nm decreased with respect to those of the other bands, suggesting a transition from a rather coplanar-like fluorene-fluorene confomation to a more twisted conformation.

Adriana Pietropaolo
University of Catanzaro,
Department of Health Sciences

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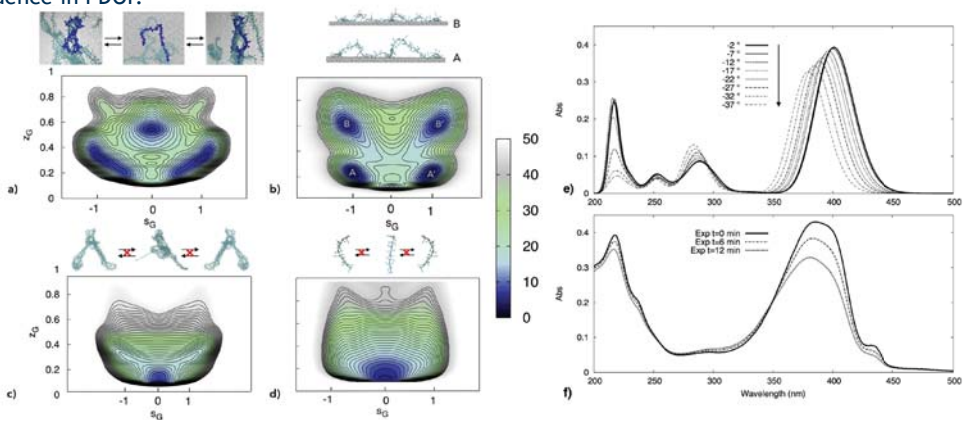


Free-energy profiles of the achiral-to-chiral transition of PDOF. a) Sixteen chains of PDOF deposited on amorphous silica, b) one chain of PDOF deposited on amorphous silica, c) sixteen chains of PDOF in vacuum, and d) one chain of PDOF in vacuum. Chain models corresponding to the chiral switch cycle (a) and those corresponding to the anchoring of PDOF on amorphous silica (b) are shown on top of the panels. In a), where the chiral cycle can occur, the free-energy basins in the main panel correspond to the models shown in deep blue. A schematic picture of the forbidden transition is also reported in panels c and d. e)-f) UV spectra calculated for 2,2'-difluorenyl as a function of the fluorene-fluorene dihedral (e) and experimental spectra observed on chirality induction (f). The value of -37 degree corresponds to the twist adopted in the 2,2'-difluorenyl ground state.

ISCRA

Drug delivery by mesoporous silica for skin applications: static and dynamic DFT-D2 simulations of anti-fungal drugs on amorphous silica surfaces

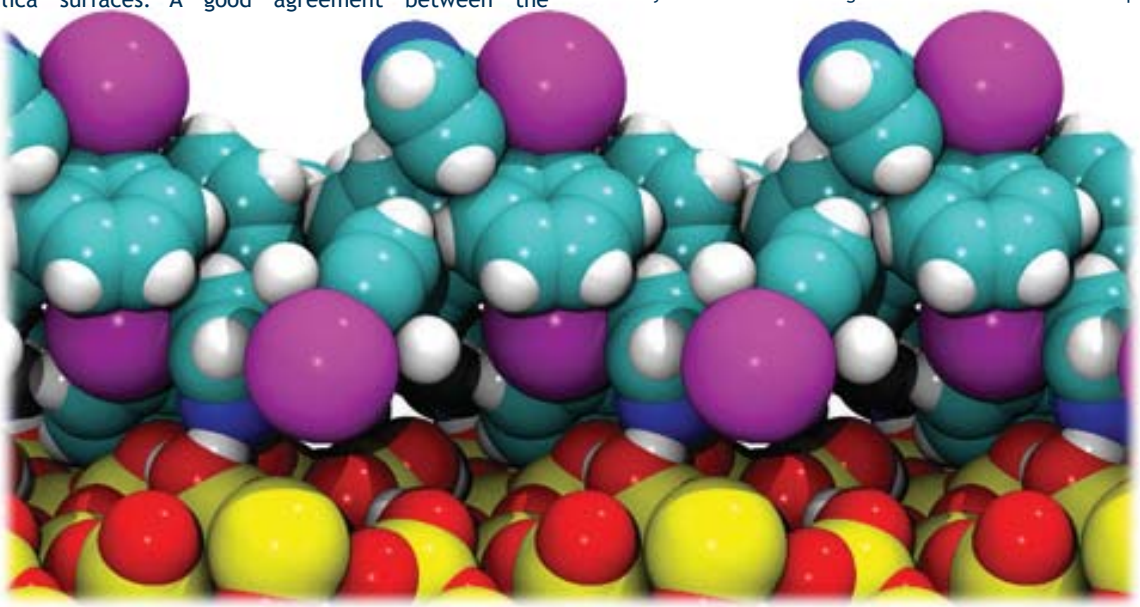
The delivery of drugs in the organism through nanocarriers is a topic of great interest in pharmaceutical research. An efficient Drug Delivery System (DDS) protects the drug from degradation, targets the diseased tissue and controls drug release. Among materials employed for drug delivery, silica plays a key role, particularly in its ordered mesoporous form. Although much research has been performed on the topic, the understanding of the interactions occurring between the material surface and drug molecules is still scarce, despite this knowledge is essential for determining the final performance of a DDS. Molecular modeling can give a precious insight on this issue, acting as a virtual microscope to study the processes occurring inside the carrier.

In this ISCRA-B project, we characterize the incorporation of clotrimazole, a common antifungal drug, inside ordered mesoporous silica by means of a joint computational and experimental approach. Modelling involved static and dynamic Density Functional Theory simulations of clotrimazole adsorbed on realistic models of amorphous silica surfaces. A good agreement between the computational and experimental results was obtained, concerning the energies of adsorption, the infrared spectra and the distribution of drug inside the mesopores. A complete interpretation of the experimental results was possible only when simultaneously considering all the complex aspects of the drug-silica interaction. These results suggest that similar ab-initio simulations can be used to predict the behavior of drugs inside the pores of mesoporous silica materials.

Massimo Delle Piane, Marta Corno, Piero Ugliengo
University of Torino, Department of Chemistry

Andrea Gignone, Barbara Onida
Politecnico of Torino, Department of Applied Science and Technology

Monolayer of clotrimazole drug molecules adsorbed on an amorphous silica surface.



Magnetic properties of strongly interacting matter

Quark-Gluon Plasma (QGP) is a new state of matter which is believed to be formed when strongly interacting matter is heated at temperatures far exceeding one trillion degrees, i.e. above the so-called deconfining temperature Tc, where quarks and gluons start to be effective degrees of freedom of the system, in place of hadrons. The properties of such medium, which filled the Universe during its early stages, are still largely unknown, with a few possible suggestions coming from heavy ion collision experiments. Theoretical input comes from numerical simulations of Quantum Chromodynamics discretized on a space-time lattice (lattice QCD).
In this project, which is based on numerical simulations running on Fermi, we are exploring the magnetic properties of this new phase of matter, something which is relevant both to the early stages of the Universe and to heavy ion collisions, with predicted magnetic fields going up to 10^{16} Tesla. In previous studies we have already predicted that the QGP behaves as a paramagnet, with a magnetic susceptibility which strongly rises with the temperature [1,2].
We are now addressing the issues of non-linear corrections to the response of the medium and of its behavior below Tc. Non-linear corrections turn out to be important for magnetic fields well above 10^{15} Tesla. Results obtained at temperatures around 90 MeV (T ~ 0.6 Tc) do not still confirm the diamagnetic behavior expected for a pion gas, the magnetization being still positive or compatible with zero. That might represent an interesting challenge to the Hadron Resonance Gas (HRG) model, which is otherwise expected to well describe this range of temperatures.

Massimo D'Elia
Pisa University

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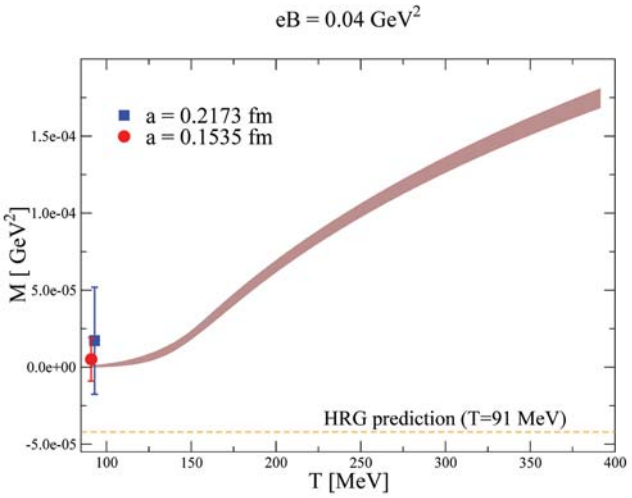
Magnetization of the strongly interacting medium at fixed magnetic background field as a function of temperature. The solid band is a continuum extrapolation obtained from our results on the magnetic susceptibility. The two data points represents direct determinations by an independent method at two different lattice spacings. The dashed line represents the HRG prediction for T = 91 MeV.



Implicit Large Eddy Simulation using the Discontinuous Galerkin method

The objective of the ILESDG project was to assess the applicability of a high-order Discontinuous Galerkin (DG) method for the simulation of under-resolved turbulence. Large Eddy Simulation (LES) bridges the gap between no (Direct Numerical Simulation, DNS) and full modelling (Raynolds-Averaged Navier-Stokes, RANS) by proposing to solve the large scales of turbulence and to model the effect of the smaller scales by adding a subgrid viscosity. Among the several LES models proposed in the literature, the Implicit Large Eddy Simulation (ILES) seems to fit well within the DG framework. In fact, while the high accuracy of DG allows to capture the inviscid cascade of kinetic energy through the inertial subrange, the natural numerical dissipation of the discretization acts like a subgrid model. The capability of the DG solver MIGALE for the ILES has been assessed in the computation of the transitional flow around a wing characterized by a laminar separation bubble. The simulations have been performed with a fifth-order linearly implicit Rosenbrock-type Runge-Kutta time integration scheme, thus exploiting the benefits of the high-order discretization both in space and time. To investigate the influence of p- and h-refinement, the flow has been computed with different polynomial DG approximations on two nested meshes. Although having far less degrees of freedom per equation, the coarse grid higher-order solution was comparable and even better than the lower-order solution on the fine mesh, thus indicating that p-refinement is preferable to h-refinement in terms of global accuracy.

Alessandro Colombo
Bergamo University

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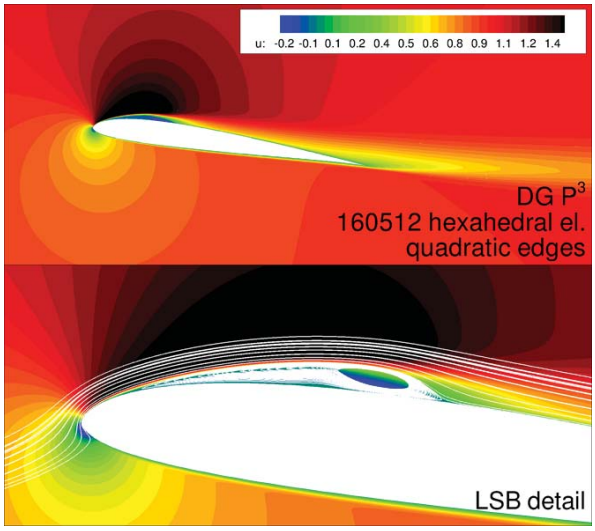

Figure 1: Contours of mean x-component of velocity with detail of the laminar separation bubble (fine grid)

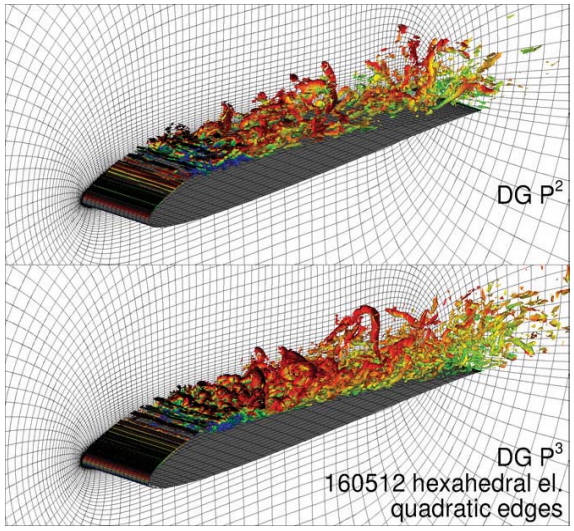

Figure 2: The use of higher-order approximations dramatically improves the resolution of the vortical structures above the airfoil as shown by the isosurface of Q-criterion (fine grid)

Turbulent drag reduction at high Reynolds numbers

Techniques for skin-friction turbulent drag reduction (DR) are the subject of intense research activity, owing to their potential environmental and economical benefit. Promising active open-loop techniques have been recently identified which leverage a wall-based forcing in the spanwise direction; prominent among them are the streamwise-traveling waves (Quadrio et al, J Fluid Mech. 2009). Our knowledge of such techniques is limited to laboratory studies or Direct Numerical Simulations (DNS) where the Reynolds number Re has a very low value and shows that their performance decreases with Re. On the other hand, in applications Re is typically very large. The current belief is thatas soon as Re becomes large enough to realistically describe an application, for example an airplane in cruise flight, the benefit would then be nearly zero.

We perform a massive numerical study which comprises more than 4000 DNS of turbulent channel flows to characterize the streamwise-traveling waves at high Re. The main outcome is that the DR is not the quantity that remains constant with Re for wall-based techniques, but the control-induced vertical shift of the mean velocity profile in the logarithmic region. Once this is discovered, DR data at moderate Re can be used to predict the amount of DR at much higher Re. DR of more than 20% can be achieved at Re one order of magnitude higher than cruise flight ones.

The present study radically changes the perspective for technological developments of drag reduction techniques, and opens interesting fundamental questions on the physics of boundary layers at higher Re.

Davide Gatti
Karlsruhe Institute of Technology (KIT)

Maurizio Quadrio
PoliMI

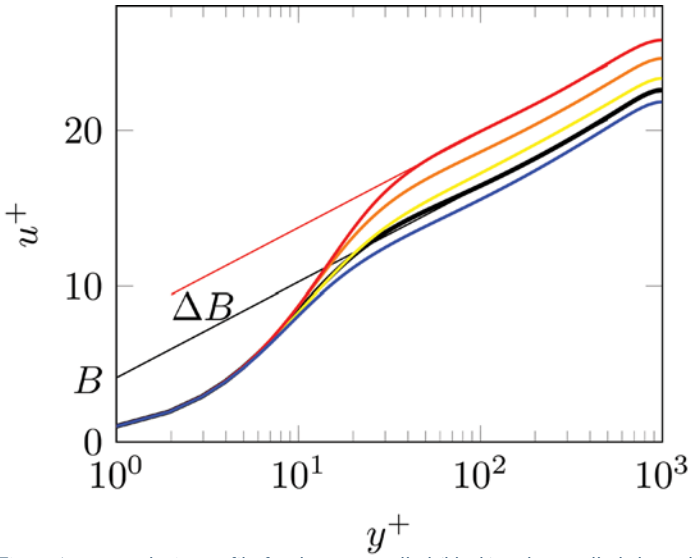

Figure 1: mean velocity profile for the uncontrolled (black) and controlled channel flow at moderate Re. The effect of wall-based control is a vertical shift of the so-called log-region.

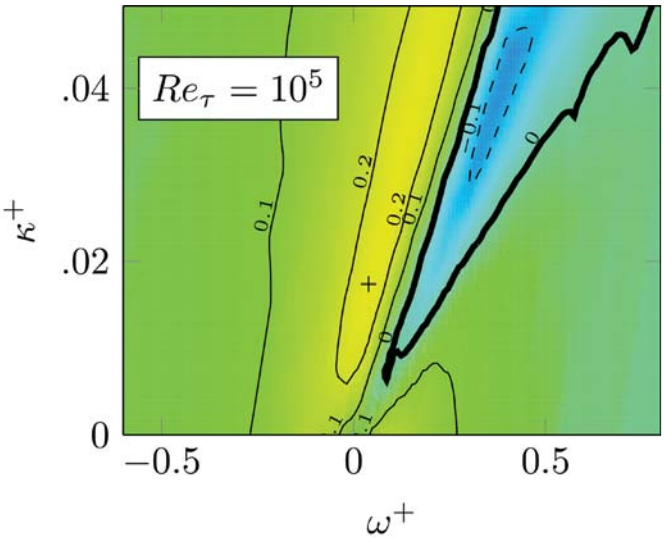

Figure 2: percent skin-friction drag reduction achievable at Reynolds number typical of a civil aircraft in cruise flight.

LISA

Simulations of electro-chiroptical and circularly polarized luminescence activity of inherently chiral conjugated polymers

Simulation of electronic properties of conjugated polymers is a major effort, which requires high and reliable computational facilities. The molecular systems under study are thiophene-based polymers with inherently chiral electroactive backbone. Different charge and spin states have been spectroscopically characterized. Density functional Theory approach (DFT) was employed in order to simulate properties like the UV absorption spectra as well as the Circular Dichroism (CD) spectra for neutral and charged species. Also the Luminescence properties, in particular Circularly Polarized Luminescence spectra, were calculated and the excited states of the simple monomeric system were characterized. In the course of the research we also defined the charges located along the oligomer backbones, as well as the bond order (defining the degree of conjugation) and bond lengths. The simulated properties have been compared to the experimental data obtained in our laboratory. Other polymers built from different structural chemical units are under study with the same electro-chiroptical spectroscopies.

Giovanna Longhi
Brescia University

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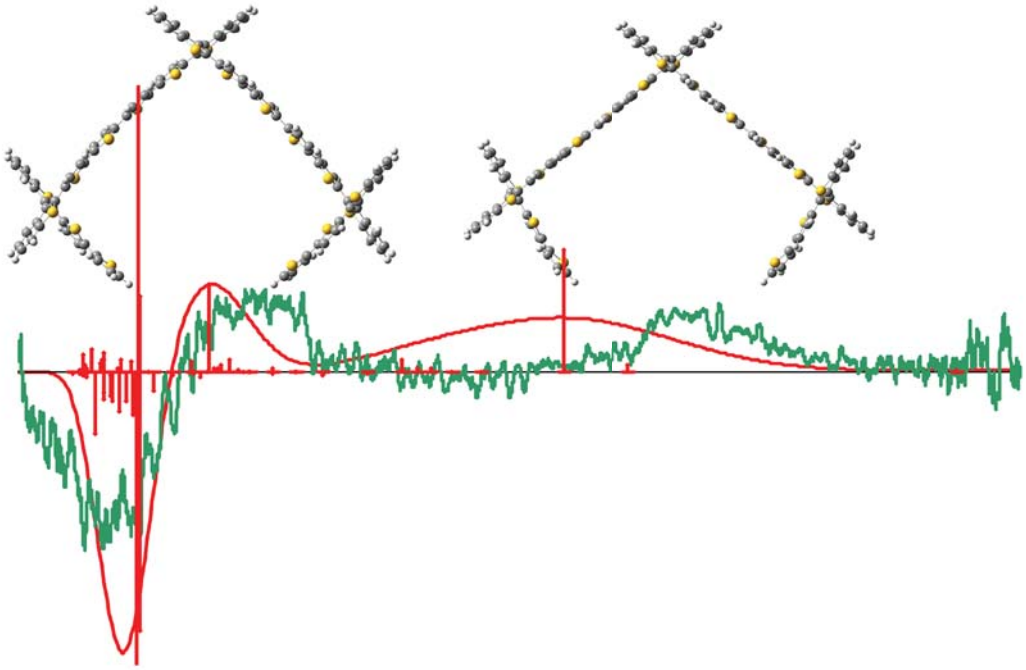
F. Sannicolò et al. Chem. E. J., 20, 15298 (2014)
Patent MI 2014A000948 "Oligoareni e oligoeteroareni macrociclici elettroattivi ad assi stereogenici"

Comparison of neutral and charged structure of a trimer synthesized from 2,2'-bis(2,2'-bithiophene-5-yl)-3,3'-bithianaphthene and experimental and calculated CD spectrum for the charged polaronic state.



LISA

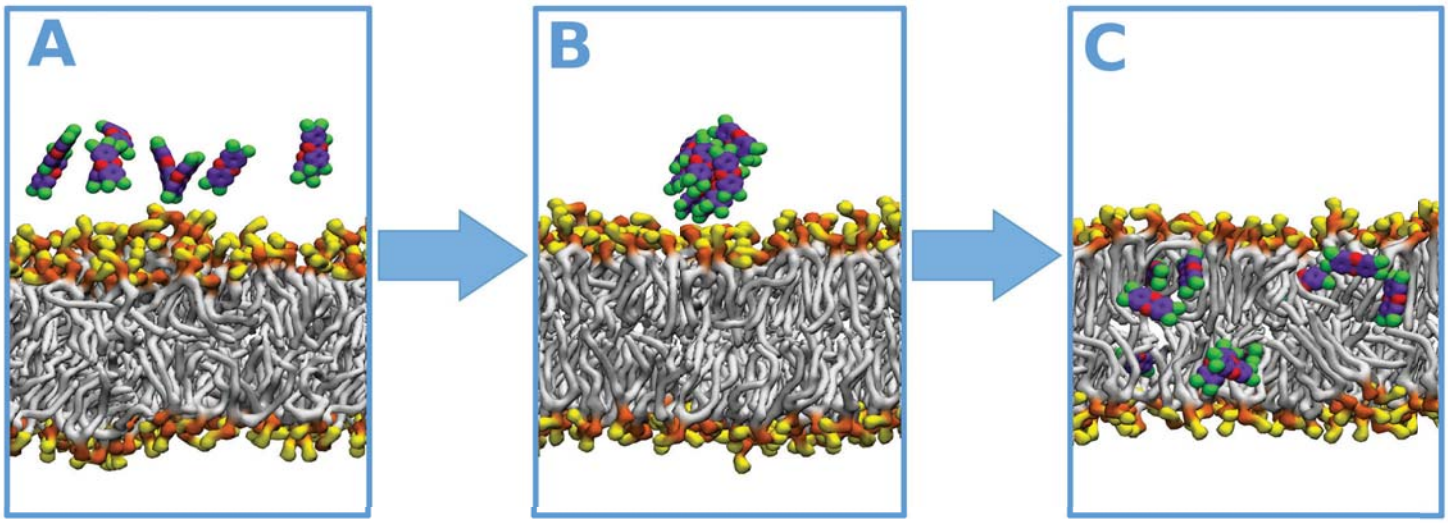
Hydrophobic aggregation and collective absorption of dioxin into lipid membranes: insights from atomistic simulations

The term 'dioxin' is commonly used to refer to a family of toxic chemicals that share similar chemical structures and induce harm through similar mechanisms of action. Overall, the dioxin family counts more than two hundred members, with 2,3,7,8-tetrachlorodibenzop-dioxin (TCDD) recognized as the most toxic. Based on the weight of animal and human evidence, TCDD has been classified as a "human carcinogen" under the EPA's draft guidelines, the other dioxins being "likely human carcinogens". Despite the large number of studies on TCDD toxicokinetics, the current understanding of how these processes occur at the molecular level is quite limited. Here, we have applied Molecular Dynamics (GROMACS-4.6 program suite) to simulate the absorption and diffusion of dioxins into biological membranes. All simulations were carried out at constant temperature (325 K) and pressure (1 atm). As an input structure for the simulations, we used a pre-equilibrated bilayer containing 128 DPPC (1,2-dipalmitoyl-sn-glycero-3-phosphocholine) molecules in water. Our results show that TCDD absorption is a spontaneous process. In water, TCDD molecules can form aggregates that quickly enter the membrane in a single step. Free energy calculations show a deep energy minimum at 1.2 nm from membrane centre and the absence of an energy barrier for TCDD permeation into the membrane.

Mosè Casalegno, Guido Raos
PoliMI

Guido Sello
Milano University

MD snapshots showing the absorption of 10 TCDD molecules. The molecules, initially separated (A), aggregate to form a cluster (B), which is quickly absorbed (C) by the membrane.



Headquarters:
Via Magnanelli, 6/3
40033 Casalecchio di Reno, Bologna, Italy
Tel. +39 051 6171411

Via R. Sanzio, 4
20090 Segrate, Milano. Italy
Tel. +39 02 269951

Via dei Tizi, 6/B
00185 Roma. Italy
Tel. +39 06 444861

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