Cineca HPC Report

the Italian cutting-edge HPC platform

HPC for public and industrial research

technical support and consultancy

applications co-development

customized data solutions

cloud services

CINECA SCAI

SuperComputing Applications and Innovation

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Cineca HPC Report

2013

Dear Colleague,

Welcome to the Cineca HPC Report, a source of information that I hope will become a regular appointment between Cineca and all its stakeholders, to make you more and more involved in our vision, in our perspective of development and in our activity at large.

The period we describe in this report has been full of activities, and challenges arising from the complexity that the globalization and the worldwide competition pose at national and European levels in the international scenario, of which Cineca is a renowned player, but also with much satisfaction in achieving outstanding goals.

The installation and the full production of Fermi, the Italian PRACE Tier 0 supercomputing system, which entered the Top500 at no 7 in June 2012, the design and implementation of Eurora, the high energy efficiency prototype funded by PRACE, the result of a successful collaboration between Cineca, INFN and Eurotech, the technology provider of this project, several structured collaborations of great relevance and impact with the major national research institutes, the permanence in a leading position in the most relevant European HPC initiatives are some of the goals we have pursued and achieved, and reported in section 2 of this publication.

The third section of the report is for us the most important. It represents the concretization of the vital activity of the department, the support to the computational sciences scientific community. We like to think that it is also thanks to the existence of a state-of-the-art infrastructure such as ours and of a highly skilled support, that so many excellent projects have been able to give ground breaking scientific results, and therefore we are glad to present some of them, the idea being to even increase, strengthen and broaden our support to the national and the European scientific community.

All the above and more are covered in this report; I would like to thank in particular the Cineca Top Management and its Governance, all my Cineca colleagues for the great job they do every day, for their enthusiasm and for making all of this possible, as well as to the Cineca Scientific Committee for PRACE and the Italian scientific community for their continuous support.

Sanzio Bassini

Director of SuperComputing, Applications & Innovation Department of Cineca

Courtesy of Matteo Bernardini, Department of Mechanical Engineering and Aerospace, University of Rome "La Sapienza".
Animation of the flow field generated by the interaction of a normal shock wave at Mach 1.5 with the Cineca logo.

SECTION 1 Overview

Cineca Mission, Governance and Management Structure

Cineca is a non profit Consortium, made up of **69 Universities and 3 Institutions**, and today is the largest Italian supercomputing centre. With more than seven hundred employees, it operates in the technological transfer sector through High Performance Computing and High Performance Data Analysis, management and development of networks and web-based services, and development of complex information systems for treating large amounts of data. Today Cineca is the high-technology bridge between the academic and research world, and the world of industry and public administration.

Cineca (whose President is Prof. Emilio Ferrari and General Director is Dr. Marco Lanzarini) is organized in 9 departments which collaborate in a constant exchange of skills and resources. The department in charge of HPC and HPDA is SCAI, SuperComputing Applications and Innovation Department, led by Dr. Sanzio Bassini and organized as shown in the next page diagram, in 5 teams.

The **Task Force for the Strategic Development** was created for exploring and concretizing new opportunities of collaboration, partnerships, new architectural projects, new industrial services, new projects for the HPC ecosystem development and for the participation in the EC programme Horizon2020.

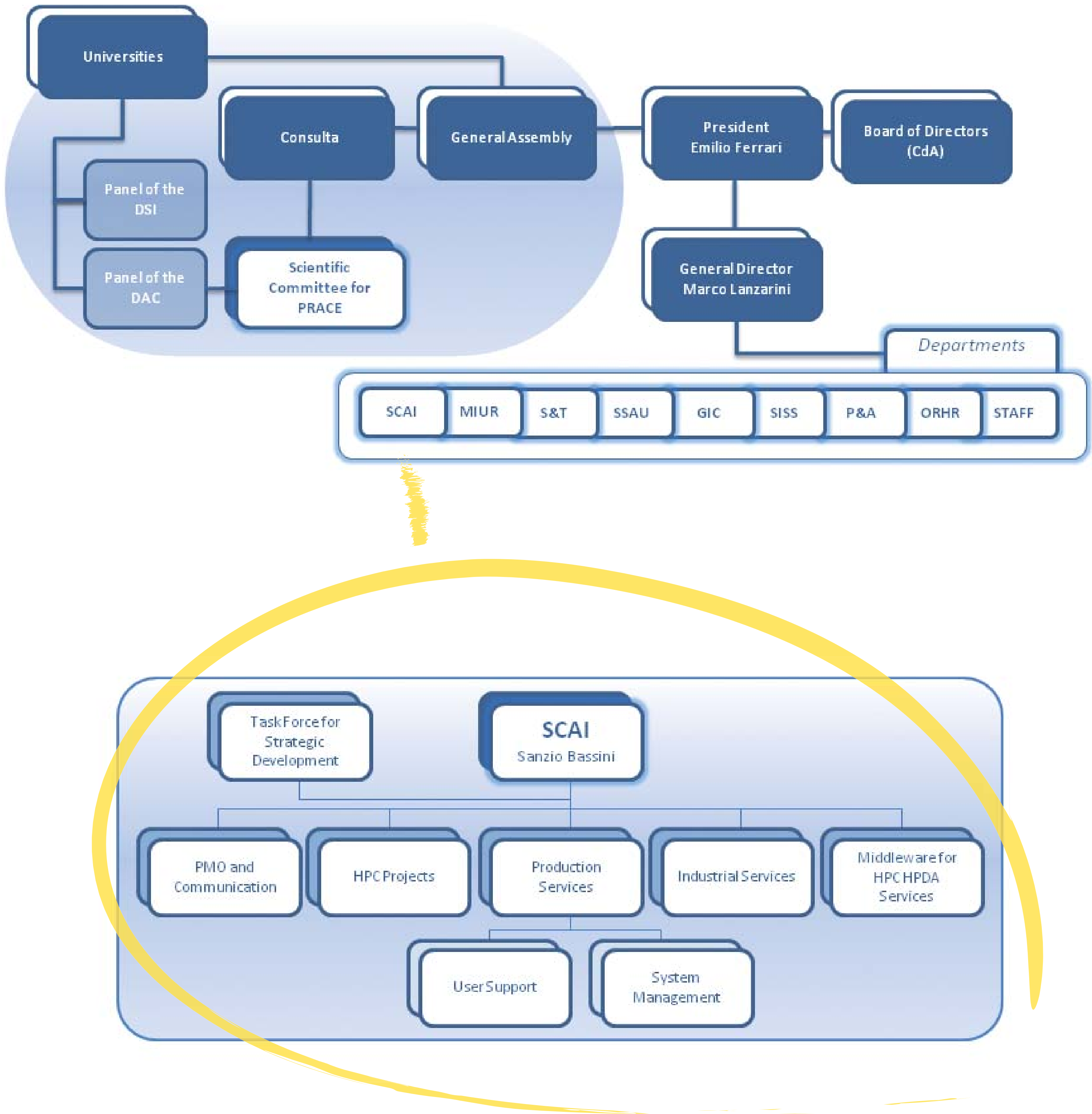
The **PMO and Communication Team** is in charge of the financial, administrative and day-by-day management of the SCAI projects. The access programmes ISCRA, LISA and (the national support for) PRACE are managed by the team as well as all the communication and outreach aspects of the department.

The **HPC Projects Team** is in charge of the implementation of all the initiatives, funded by European, national and local entities, aiming at the exploitation of the HPC infrastructure.

The **Production Services Team**, with its two operational units (User Support and System Management) is responsible for all the processes related to the management and maximization of the production of the infrastructure: systems, storage and network administration, workload and applications management, basic and specialistic support, both for public research and for industrial and private customers.

The **Industrial Services Team** is in charge of all the contracts and the developmpent and technology transfer actions with private and public customers, big industries and SMEs.

The **Middleware for HPC-HPDA Services Team** is responsible for the development and the deployment of the services for access to the HPC and data infrastructure.


Universities
Consulta
General Assembly
President
Emilio Ferrari
Board of Directors
(CdA)
Panel of the
DSI
Panel of the
DAC
Scientific
Committee for
PRACE
General Director
Marco Lanzarini
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Strategic
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Sanzio Bassini
PMO and
Communication
HPC Projects
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Industrial Services
Middleware for
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User Support
System
Management

Cineca: a Success Story for more than 40 Years

Identifying high performance computing in Italy is quite easy: Cineca.

Describing HPC in Cineca means recounting a long success story.

Starting from 1969, when the Ministry of Education supported four universities in the effort of consortiating and creating a supercomputing center in Bologna with the CDC 6600, the first system designed by Seymour Cray, today, after the merging of the three Italian consortia Cineca, Cilea and Caspur, with a unique national consortium of multiple sites, Bologna, Rome and Milan, the story of Cineca is a succession of challenges faced and overcome, with the major aim of supporting Italian research.

For 44 years, Cineca and its HPC department have been leaders in Italy in the deployment of a solid and trustable HPC environment, being the reference point for the national academic and research system, and conveying the most advanced technical and scientific expertise in its young and multi-disciplinary staff.

Remarkable achievements in the last years include a big series of long-term strategic partnerships with outstanding national research entities (INFN, SISSA, INAF, INGV, OGS) accelerating the scientific discovery and the technical development of high performance computing, plus a gained forefront position in Europe, becoming one of the four PRACE Tier 0 sites, thanks to a forward-looking attitude of trust of the Ministry of Education, University and Research and a constant presence of Cineca in the main European initiatives and discussion tables on HPC.

A milestone in the long success story has been undoubtedly the world-class system Fermi, the BlueGene/Q that took the no. 7 position on the June 2012 Top500 ranking list and defended a top ten ranking for many months until June 2013; an even more recent milestone is the installation in Cineca of the Eurotech system Eurora, the PRACE prototype deployed by Cineca and INFN, #1 in Green500 list (June 2013), offering the most efficient technology for hybrid HPC system.

A involvement of Cineca in the Human Brain Project, in EUDAT and other initiatives like the RDA (Research Data Alliance) aiming at accelerating progress on the data management and on the sharing of open research data to drive innovation, in parallel with national initiatives in bioinformatics like Epigen, towards the creation of a center of competence, and the European Technology Platform for HPC for driving the technology development, the collaboration with Intel leading to the recent appointment of Cineca as Intel® Parallel Computing Center, for the parallelization of codes like Quantum ESPRESSO and SPECFEM3D, represent only some of the challenges faced nowadays, on the way towards Italian and EU growth, competitiveness and innovation.

Prof. Francesco Profumo, Italian Minister for Education and University,
between Dr. Marco Lanzarini and Prof. Emilio Ferrari, General Director and President of Cineca, at the inauguration of Fermi, in Cineca.

Dr. Kostas Glinos, Director of the European Commission DG CONNECT, Dr. Sanzio Bassini, Director of SCAI Department at Cineca,
Ms. Catherine Rivière, Chairman of PRACE and CEO of GENCI,
Prof. Thomas Lippert, Coordinator of the Human Brain Project and Head of Jülich Supercomputing Centre.

2nd EUDAT Conference, Rome, 28-30 October 2013. 215 participants joined this international event from more than 18 countries and many institutions represented coming from academic research, international bodies, public administration, industry and media.

The SCAI staff at the Cineca booth, SuperComputing2012, Salt Lake City, November 2012.

Cineca and its Strategic Role in HPC

The European Commission document "HPC: the Europe's place in the global race" (2012) states that High Performance Computing (HPC) is an important asset for EU innovation and stresses its strategic importance for EU industry and research, as well as for its citizens, by supporting the development of innovative industrial products and services, increasing competitiveness, and addressing societal and scientific grand challenges more effectively.

In June 2013, the European Competitiveness Council endorsed the document, and adopted a resolution stating that HPC must be ranked as a top priority in the Horizon-2020 framework programme.

HPC has become increasingly a fundamental instrument to advance scientific research; computational methods became a research paradigm alongside theoretical speculation, observation and experiment.

Cineca, also thanks to forward-looking vision of the National Minister of Education, University and Research, provides the public and the private Italian research ecosystem with access to the most advanced computing systems available, playing a strategic role in this context.

Key goals, constantly reinforced, are:

- access to state-of-the-art HPC resources by the computational science community in Italy,
- direct access to HPC-driven technologies by companies active in strategic sectors like energy, security, aerospace, environmental risk management and cyber-space, supporting the innovation processes for competitiveness,
- a strong educational effort to develop HPC competences and skills and make them available to academia and industry.

Because of Cineca's activities, the Italian HPC ecosystem demonstrates significant strengths, thanks to many elements of excellence, internationally acknowledged, present at scientific, academic and industrial levels:

- the current production supercomputing system, the Fermi Blue Gene / Q, was ranked in the top ten of the Top500 list just one year ago, at the time of its initial deployment;
- Cineca is a Tier 0 Hosting Member of the PRACE European supercomputing infrastructure;
- a recent high energy efficient prototype co-designed by Cineca experts was ranked #1 in the June 2013 Green500 list;
- a well established open access peer-reviewed programme guarantees to the Italian and European scientific community high quality HPC service provision.

The action of Cineca is valuable, both in the local scenario, where the Consortium represents the National Supercomputing Facility, and in the international and European scenario, where Cineca plays a key role. New strategic challenges are posed by the continuous technological innovation process, such us:

- ensuring long term continued access to state-of-the-art HPC computational resources for scientific and industrial users, at the Tier 0 and Tier 1 level;
- ensuring that one top level (Tier 0) HPC infrastructure is constantly available in the country (e.g., within the first ten entries of the Top500 list);
- supporting and strengthening the available know-how in HPC;
- ensuring that all competences available in Italy are fully acknowledged and rewarded as the national contribution to the European HPC effort.

To address such a competitive scenario, Cineca should rely on a closer interaction and collaboration with its stakeholders. Not only a service provider, which remains the main stream of the Consortium mission, but also a point of reference - or center of competence - for supporting a wide scientific, academic and industrial (SMEs in particular) community in the best usage of HPC technologies and a strong effort in high level specialized education and training programmes.

To this end some remarkable actions have been consolidated.

A strong collaborative agreement has been signed with INFN, to make available to the astro-particles community a supercomputing system at a very early stage of deployment and transfer the accumulated experience of the INFN scientist to other scientific communities, helping Cineca in the exploitation of new generations systems; for example the Fermi system, one of the first BG/Q machines in a large configuration available for intensive production worldwide, or the exploitation of the floating point accelerators (GPU and / or Intel Xeon Phi) in a hybrid configuration.

Also by means of the financial support from the Minister, an aggregation of competence has been created in the Italian northeastern area, based on a formal collaboration agreement between Cineca and National Institute of Oceanography and Experimental Geophysics in Trieste, including ICTP and SISSA-ISAS.

Within the academia, besides the already mentioned SISSA-ISAS collaboration, a strong link has been forged with University of Florence and the European Laboratory for Non-Linear Spectroscopy, to collaborate in the Human Brain Project, and with the University of Bologna and University of Padua for the architectural design of a high-energy efficient HPC solution.

All with the ultimate objective to create with the Cineca stakeholders a Center of Excellence, competitive at a European level and essential for the whole Italian public and private research system.

Cineca
national collaborations

SECTION 2
Service
Provision

Cineca and its SuperComputing Infrastructure: our Recent History

In 2008 Cineca, for 40 years a key-player in the field of HPC, started the project that led to the 100 TeraFlops machine, an IBM Power6 (named SP6) with AIX. That implied, as a first step, to convert the smaller of the two HPC machine rooms in a liquid cooled location.
This project brought also in the air cooled machine room one rack of an IBM Blue Gene/P system (devoted primarily to Italian and international researchers for scientific simulations) as one of the possible technological evolutions to move to the PFlops scale.
In 2012 Cineca moved to a PFlops system FERMI, an IBM Blue Gene/Q.
The refurbishing of the liquid cooling circuits required only few changes, given that the power and cooling needs of the system were the same of the predecessor Power6, even though the computing performance is 20 times higher. The savings in energy and funds were re-invested to increase the computing and storage capacity.
Thanks to this careful resource management, Italy, with FERMI@Cineca, stayed ranked for the whole of 2012 among the ten most powerful High Performance Computers in the world.
In addition, the system for technical computing, an IBM Dataplex air cooled linux cluster, named PLX, drives important technical simulations from national and international private companies, as well as the weather forecast models for the Civil Protection agency. Reinforced and upgraded in 2011 it is now composed of more than 3000 cores (with GPUs).
Maintaining its tradition of advanced computing and innovation center and in collaboration with the European initiative PRACE, Cineca in 2013 installed a Eurotech “production prototype”, EURORA, derived from the Aurora technology. EURORA is a 64 node linux hybrid cluster equipped with the most recent and powerful CPUs and GPUs. It is a hot water cooled system, powered with direct current. Although not very large it is a very efficient system, ranked #1 in the Green500 list (June 2013). Its energy efficiency improves upon the previous greenest supercomputer in the world by nearly 30%.
This powerful computing infrastructure produces a huge amount of valuable data that needs an appropriate repository to store it. After a first step towards the creation of a complex infrastructure where to preserve, process and manage enormous datasets, (namely the installation of a DDN SFA10K storage system with 500 disks for a total amount of 900 TiB of raw disk space), a tender for dramatically enlarging the capacity and the access performance to the repository has been launched.
With the outputs of this tender Cineca is actually becoming a powerful and complete infrastructure able to support and push the competitiveness of the Italian and European private and public research.

EURORA - Eurotech Aurora
at Cineca

Strengthening the European HPC Infrastructure

Since the beginning of the 3rd Framework Programme, Cineca has played a role at European level, being active in different European projects both, at research and infrastructure levels. The core is represented by the PRACE Implementation Phase Projects, aimed to sustain the action of gathering leadership-class HPC systems and competences as a single infrastructure, available to all researchers in Europe, to keep them at the forefront of discovery. In PRACE-1IP, 2IP and now PRACE 3IP Project, Cineca activity focuses on:

• the management and the evolution of the distributed supercomputing infrastructure connecting the Tier 0 and Tier 1 sites, as well as the definition and implementation of services and tools for user support, systems management, and security policies;

• the enabling and peta-scaling of applications of interest for the scientific communities: the work on Quantum ESPRESSO for materials science, GROMACS for molecular dynamics, SPECFEM3D for geophysics and OpenFOAM for CFD etc, establishes a patrimony for the scientists that goes well beyond the PRACE project, contributing to the growing of a consolidated European HPC infrastructure;

• the provision of advanced training courses in HPC which placed Cineca as one of the six PRACE Advanced Training Centres (PATCs);

• the evaluation of innovative energy efficient solutions for peta-scale HPC systems, leading to the co-design and testing of the prototype EURORA;

• the set up of a pre-commercial procurement (PCP) for a 'Whole System Design for Energy Efficient HPC'. The action is the first of this kind in Europe and gathers a group of five PRACE Partners as procurers, coordinated by Cineca.

HPC adoption from industries, and SMEs in particular, is an important target at European level and Cineca is deeply involved in this action, strengthening the relationships with industrial users. Within PRACE Cineca leads the SHAPE (SME HPC Adoption Programme in Europe) pilot to demonstrate to a few selected SMEs how to overcome barriers in the access to HPC and how HPC technologies can help to improve their production processes and to foster innovation. Furthermore, Cineca is a partner in FORTISSIMO, “Factories of the Future Resources, Technology, Infrastructure and Services for Simulation and Modelling”, aiming at enabling European manufacturing to benefit from the efficiency and competitive advantage inherent in the use of HPC simulation. Fortissimo aims at the provision of simulation services running on a cloud infrastructure making use of HPC systems, making also appropriate skills and tools available in a distributed, internet-based environment.

These projects contribute to further consolidate the Cineca HPC infrastructure integrated with the Data Infrastructure (important here is the role of the EUDAT project aiming to build a European Data Infrastructure) harmonizing it at the European level, for the benefit of scientific communities. An example of using such infrastructure is represented by the Earthquake and seismology research community where, thanks to the VERCE project, scientists can experiment a suitable platform for HPC and data intensive simulations.

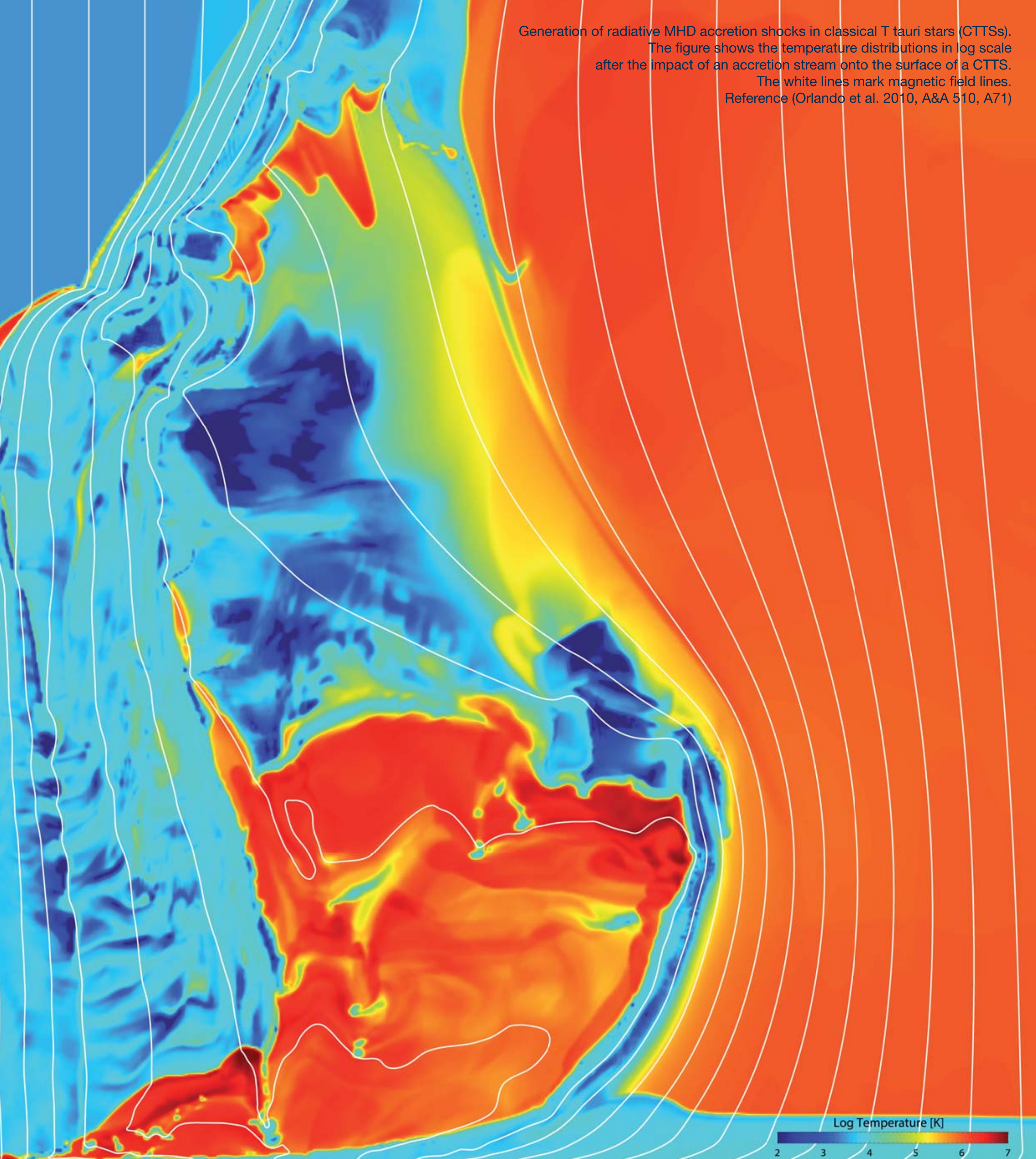
The technological evolution and the increasing computational demand lead to a new generation of computers composed of millions of heterogeneous cores which will provide extreme performances, in the range of Exascale, around 2020. Europe is fostering the evolution of HPC infrastructure toward Exascale, funding ad-hoc projects to address innovative Exascale enabling supercomputing platforms. Cineca is partner in two of these, DEEP and Mont-Blanc, and their continuation DEEPER and Mont-Blanc 2, with the main task of enabling grand challenge computational applications for these prototype architectures, highly relevant for European science.

The exascale roadmap leads to software challenges that need to be addressed. Cineca, with EESI 2 (European Exascale Software Initiative 2 Towards exascale roadmap implementation), cooperates in the software roadmaps and recommendations, detecting disruptive technologies, addressing cross cutting issues in numerical processing and software engineering, developing gap analysis methodology towards Exascale roadmap implementation.

Understanding the human brain, one of the greatest challenges facing the 21st century science, is the goal of the Human Brain Project (HBP), one of the two flagship projects (the other is Graphene) funded by the EU with a lifespan of 10 years.

Cineca is a partner in HBP, involved in the HPC platform which aims to provide the HBP and the wider European Neuroscience community with the supercomputing, Big Data and visualization capabilities, necessary to create, simulate and analyze multi-scale models of a complete human brain. Cineca represents one of the four HPC infrastructures in support of the HBP activity implementing the HBP Massive Data Analytics Supercomputer, to investigate, analyze, manage and preserve the huge amount of data generated by the HBP.

All these projects, in which Cineca plays an active role, are fundamental and must evolve addressing new actions in Horizon 2020, to consolidate and further enhance the European HPC and Data infrastructure at the service of scientists, to foster new scientific challenges.



Generation of radiative MHD accretion shocks in classical T tauri stars (CTTSs).
The figure shows the temperature distributions in log scale
after the impact of an accretion stream onto the surface of a CTTS.
The white lines mark magnetic field lines.
Reference (Orlando et al. 2010, A&A 510, A71)

Access Programmes for Researchers

One of the missions of Cineca is to allow Italian and European researchers to have access for free to leading-edge computational resources. In one year of activity, starting from summer 2012, the infrastructure of Cineca made a considerable amount of computing time available, on the three systems devoted totally (FERMI and EURORA) or partially (PLX) to the academic and public research. More then 1 billion core hours on FERMI BG/Q, 9 million on PLX iDataPlex and 1 million on EURORA (in production from May 2013) were delivered to national and worldwide researchers who have benefited from the three allocation programmes available.

PRACE (Partnership for Advanced Computing in Europe), ISCRA (Italian SuperComputing Resources Allocation) and LISA (Interdisciplinary Laboratory for Advanced Simulation) are the three frameworks, strictly based on a peer-review system with two calls per year, by which scientists and engineers from Italy and Europe can have access to the most advanced, powerful and integrated digital resources and services for scientific discovery.

PRACE, dedicated to all researches worldwide, is the pan-European programme suitable for large-scale, computationally intensive projects, giving access to the European most powerful HPC systems, in Italy FERMI.

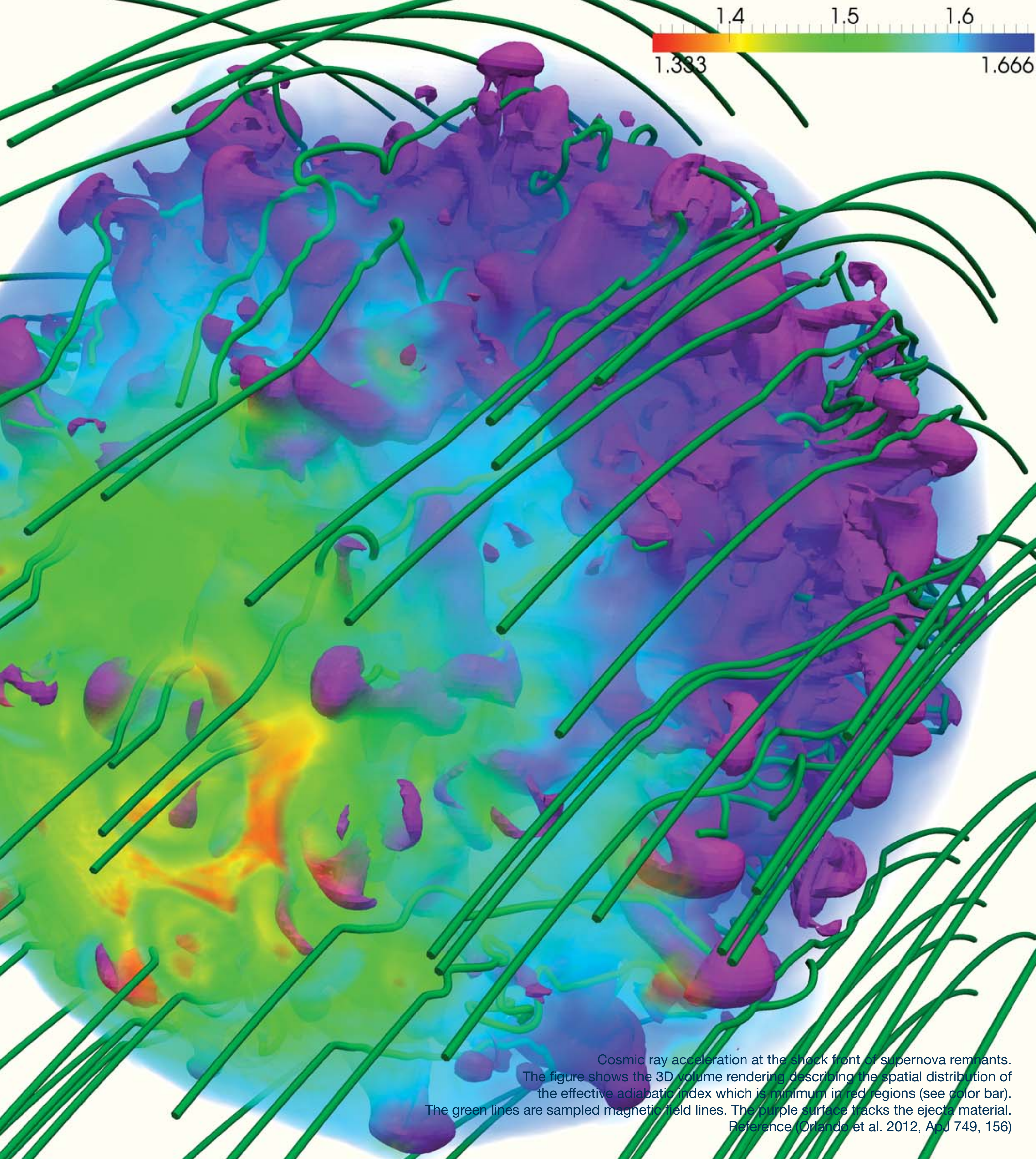
PRACE awarded in the first 7 calls for projects a total of 241 projects. Out of 241, 63 project had a PI with an Italian affiliation, an impressive 26% of all projects. More than a half, 35 of these 63 projects, were served by FERMI, while the others run on other PRACE Tier 0 systems. Regardless the affiliation of the PI, starting from summer 2012, FERMI hosted 52 PRACE projects in total.

ISCRA is the Italian SuperComputing Resource Allocation initiative, created to ensure an adequate supply to national scientists and engineers for HPC-related research. The scale of the projects is smaller than PRACE and, since its initial implementation in 2010, ISCRA received 1294 applications, of different typologies. Out of these, a total of 1055 were awarded, 59 large projects, 337 medium-size projects and 659 preparatory or trial projects. 1.015 billion core hours were allocated by ISCRA, starting from 2010 on SP6 and then FERMI, PLX and EURORA.

To support and strengthen the talent to produce technological innovation and to increase the attraction of the Lombard territory through the exploitation of expertises and platforms for numerical modelling tools, the Regione Lombardia started from 2010, with Cilea first, now merged in Cineca, a joint effort named LISA, Interdisciplinary Laboratory to Advanced Simulations.

LISA is the third Cineca access programme, dedicated to PIs affiliated with academic and research entities located in Lombardy. From January 2013 LISA received 94 applications of which 71 were awarded, for approximately 65M core hours.

These 3 programmes are an effective and trustable means to enable researchers to execute big numerical simulations on important HPC computational resources and to ensure an adequate support to Italian and European scientists and engineers in their HPC-based activity.



Cosmic ray acceleration at the shock front of supernova remnants.
The figure shows the 3D volume rendering describing the spatial distribution of the effective adiabatic index which is minimum in red regions (see color bar).
The green lines are sampled magnetic field lines. The purple surface tracks the ejecta material.
Reference (Orlando et al. 2012, ApJ 749, 156)

Training

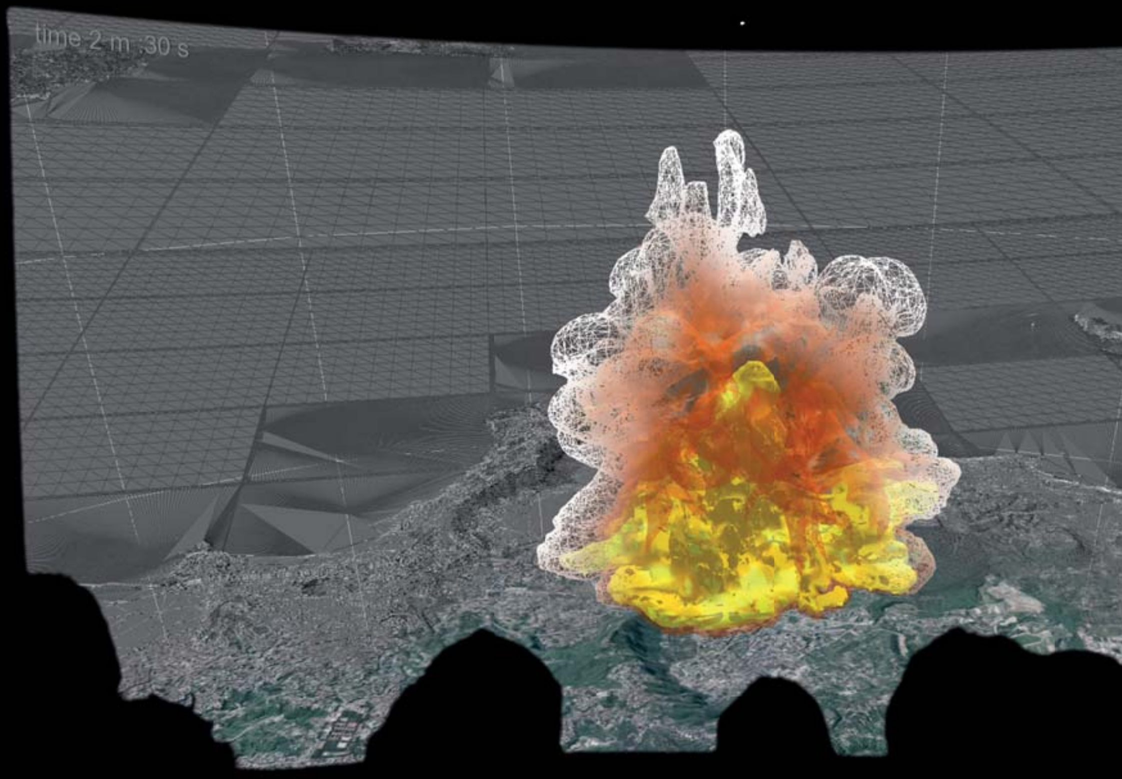
Cineca is well-known for offering a full teaching program in the field of computational sciences, to guarantee a suitable support to scientists who need an advanced training to compete in their research fields.
This knowledge is available to users by means of a comprehensive offer of consultancy services and specialized training paths. A huge number of training events are organized every year to enable users in the usage and exploitation of the available technologies and architectures.
The Cineca HPC Department, SCAI, is also one of the 6 PRACE PATCs (PRACE Advanced Training Centres) that enable the European research community to utilize the computational infrastructure available. Therefore Cineca's training offer includes several events sponsored by the PRACE-2IP European Project, labeled as PATC events.
In 2013 SCAI provided 25 courses in different editions for all the three Cineca sites (Bologna, Roma, Milano) covering 10 main topics and 7 Schools covering 5 main topics all free of charge. More than 670 Italian and international students were hosted for a total of about 140 days of lessons.
Cineca also collaborates continuously with some vendors in exploring and testing new technologies for HPC, e.g. NVIDIA GPU, Intel MIC.
The SCAI training program consists of courses, schools and workshops.
The courses are tailored to all researchers who need to build or update their knowledge on computational sciences. Lessons are held by internal experts and include access to Cineca computing systems. They are usually 2 to 4 days long and consist of theoretical lessons and practical sessions where teachers support the students to resolve prepared exercises.
Courses are targeted of 3 levels: basic, intermediate and advanced but some of them are "general-purpose" to try to give the audience a global vision of a particular topic covering arguments of all the three levels and referring to other courses for the follow up.
Schools are the traditional training events. Cineca offers on-site summer and winter schools focusing on "Parallel computing" and "Scientific visualization", both proposed on two different levels: introductory and advanced.
Introductory level schools are intended for new users, with the goals of removing the obstacles typically encountered by new users of such complex systems. Advanced schools and courses are targeted towards more experienced users and cover a range of topics related to new technologies, performance/programming tools, among others.
For some courses and for all the schools, some grants are available and are given to all students that are not funded by their institutions and working in an institute outside the site of the courses.
Occasionally, SCAI organizes some workshops on hot topics for computational science.
The web site for the SCAI training offer is http://www.hpc.cineca.it/content/training

Courses in 2013

- HPC Numerical Libraries
- Introduction to C Programming Language for Scientific Application
- Introduction to Fortran90
- Introduction to GPGPU and CUDA programming
- Introduction to HPC Scientific Programming: tools and techniques
- Introduction to Parallel Computing with MPI and OpenMP
- Introduction to Scientific and Technical Computing in C++
- Introduction to the FERMI Blue Gene/Q, for users and developers
- Parallel I/O and management of large scientific data
- Python for computational science

Schools in 2013

- Summer School on Parallel Computing
- Advanced School on Parallel Computing
- Summer School on Scientific Visualization
- Advanced School on Scientific Visualization
- Summer School on Enabling Applications on Intel® MIC based Parallel Architectures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8th Advanced
School on
SCIENTIFIC
VISUALIZATION
TOPICS:
TARGET AUDIENCE:
BENEFITS:
APPLICATION DEADLINE:
PRE-REQUISITES:
14 - 18 October 2013
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22nd Summer
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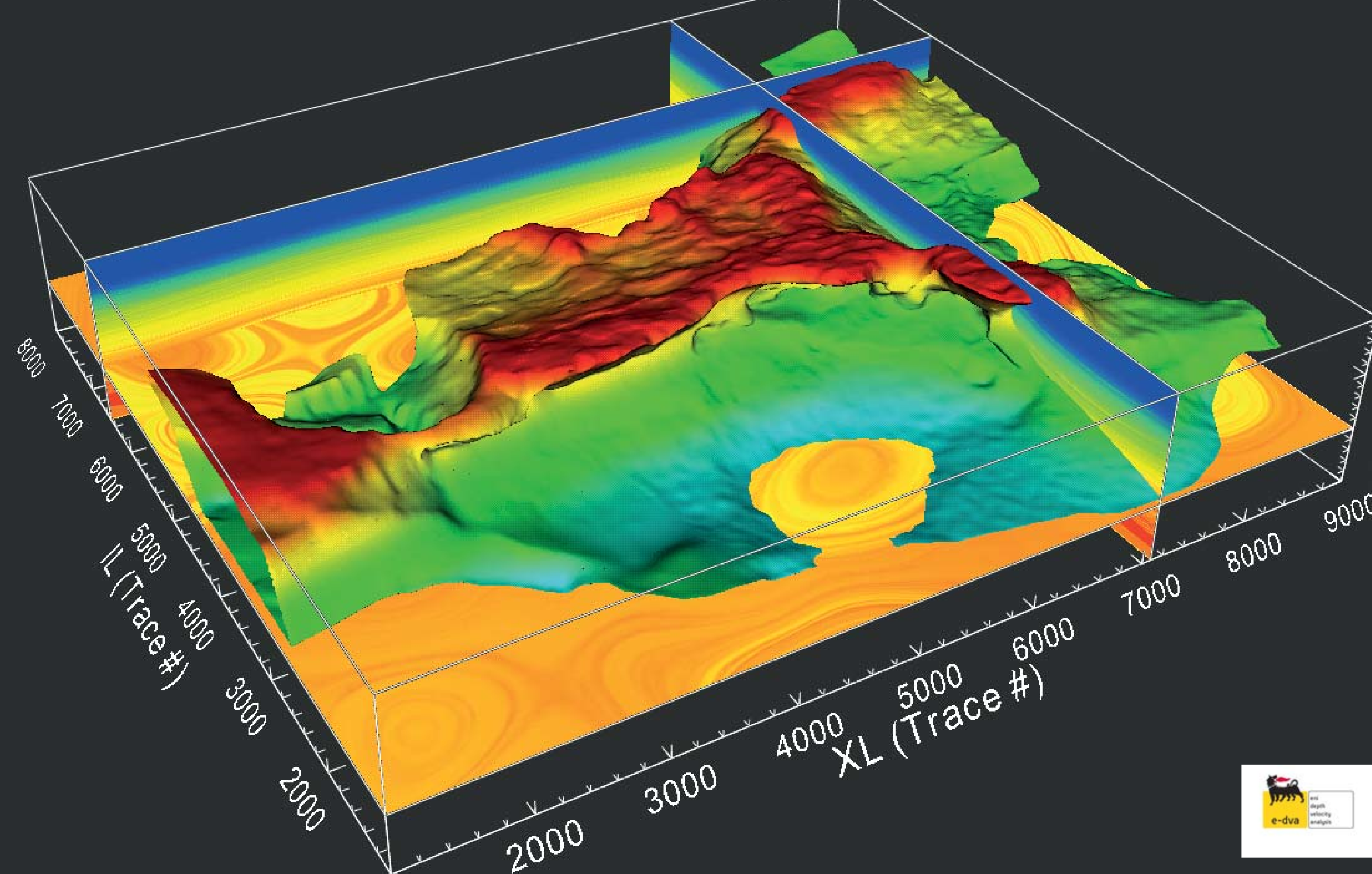
Industry

The collaboration with industry and the provision of services to industry complement and reinforce services offered to academia and to the research centers in a feedback loop improving both.
Working with industry requires, beside technical excellence, a strong commitment and focus on the production and on the Quality of the Service offered and its continuous improvement, the definition and fulfillment of the Service Level Agreements, the achievement of the project goals in the defined timeframe and the budget, and the monitoring technology trends related to the specific application or business case. This discipline can be applied to academic services improving their quality.
On the other hand working with Academia allows to look ahead for technology trends considering a wide range of applications and to experiment new programming models or HW prototypes on a wider base of applications. It also allows the testing of solutions that could be exploited and transferred to industry.
The European Commission as well as the Council of Competitiveness in US consider HPC one of the drivers for innovation. This is clearly understood by large companies but less affordable for SMEs. Therefore, the FORTISSIMO project, involving Cineca as one of the core partners, aims to deliver HPC-Cloud services to industry and to manage innovation projects with SMEs making use of the services delivered. FORTISSIMO selects through open calls and directly funds innovation projects with high economic impact. The effectiveness and return on the EC investment of Fortissimo project will be monitored and reported to EC and the public.
Large industries working in Aerospace and Oil&Gas sectors take advantage of HPC resources and technology in their production activities. In order to sustain exploration and production activities using HPC systems, Eni, the Italian largest Oil&Gas company, has established a long lasting partnership with Cineca; in the frame of this partnership Cineca offers and develops a wide range of HPC services to fulfill their requirements. The three main specialized services consist of:

- the daily management of the Eni HPC infrastructure;
- on site support to Eni users during production and management of daily needs;
- development and maintenance of HPC applications in production.

Moreover, Cineca and Eni collaborate to test new technologies, to evaluate Eni proprietary applications performance on new HW and to train Eni specialists.
Moreover Cineca offers proof of concepts and services based on ISVs applications used in different industrial sectors like automotive, finance, pharmaceutics, oil&gas, shipbuilding and CAE consulting.
Cineca not only works on technology transfer programs for industries and SMEs, but with Super Computing Solutions (SCS - http://www.scsitaly.com/), offers and operates commercial services to industry. More precisely, SCS provides a widerange of services, both for companies that have their own HPC resources in terms of small cluster and companies that don't want to buy or manage their own resources. Data Security, Service Flexibility, Remote Visualization, and HW performance are the key features of the SCS Cloud service. Customers who need fast access to resources for peak production can set up their environment and their applications, test production and get a defined amount of dedicated computing resources when they actually need them. Consulting activities on HW, system configuration and technology trends are available for those companies that want to buy their own HPC systems. SCS is available for ISVs SW testing and also CFD consulting based on OpenFOAM.



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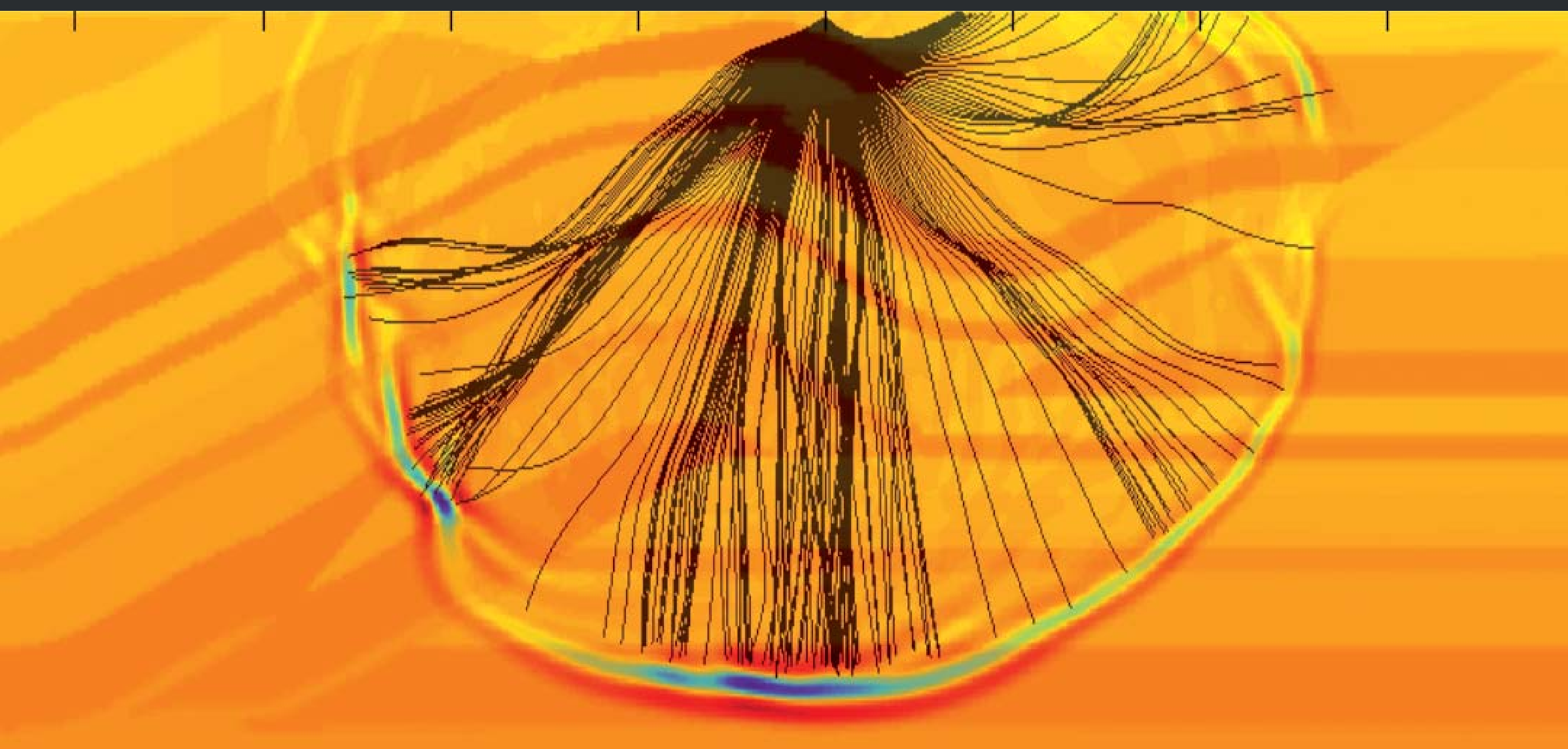


The Italian Data Panorama: Needs and Requirements

"A fundamental characteristic of our age is the rising tide of data - global, diverse, valuable and complex. In the realm of science, this is both an opportunity and a challenge"

In Italy, and more generally in Europe, it is estimated that more than 20 research institutes rely heavily on digital data. Research organizations such as INFN, INAF, CNR, OGS, INGV are running advanced data services, many of which are in international scale. With the exponential growth in data generation, whether produced by high-throughput simulations or gathered through observations, on one hand it is an extremely exciting time for scientific discovery, but on the other, institutions are increasingly feeling the pressure to develop new strategies and policies to ensure the correct management of the data generated. Data, in their various forms, represent one of the most important assets for scientific communities. However, managing data requires attention to ensure the reliability and security of this valuable asset. With the term "Scientific Big Data" it is meant the activity of collecting, organizing, storing, managing and analyzing vast amount of scientific data to accelerate discoveries in science. But digital information is inherently fragile and often at risk of loss. Access to valuable digital materials tomorrow depends upon preservation actions taken today; and, over time, access depends on ongoing and efficient allocation of resources for preservation. Cineca, in collaboration with the ICON (International Center of Computational Neurophotonics) Foundation, held a survey (spring 2013) among Italian major scientific communities (12) to obtain a quantitative picture of researchers' opinions and requirements. Here we provide a brief overview of the results, including some final recommendations.

Personal computers are still a popular place where to maintain data (Figure 2), for the 40% of researchers. However, the 76% use a centralized repository operated by their institute.

The majority of researchers (66%) appears to use data collected by others, mostly on top of data they collected themselves. However, only for the 46% of the interviewees there are sufficient possibilities of making use of other people's data. Although four out of ten researchers believe that opportunities are sufficient, it is still true that interviewees report obstacles when trying to discover other scientists' data mainly due to the lack of information about the nature of available data sources. Other reasons include problems with the quality, copyright and privacy considerations, missing metadata.

In general, researchers often agree that international solutions are required. There is also a clear trend towards planning and strengthening international research infrastructures.

The survey depicts a fragmented scenario highlighting the existence of different levels of maturity in the management of research data sets. To bridge the existing gaps, and efficiently help communities to emerge and compete on an international level, the following recommendations might represent a valuable baseline to advance the Italian data panorama:

- the availability of high speed networks linking research institutions and IT centers together, like Cineca, is fundamental to guarantee the efficient transfer of data towards computational facilities for being processed further. More important, the possibility of analyzing large volume of data in nearly real time might lead to socio-economic benefits; think to the prompt understanding of physical processes responsible for earthquakes or volcanic eruptions;
- the integration of existing data repositories, through the adoption of abstract data formats or common meta-data schema, is a key element to enable cross and multi-disciplinary research;
- it is largely recognized that preserving data close to the computational facility is the preferable approach for continuous data mining, analysis, and simulation;
- data infrastructures and services should develop gradually, and in accordance with existing solutions without imposing new standards or technology. A layer-structure based approach would guarantee the infrastructure and the community layer are independent while remaining interoperable.

The full report is on www.hpc.cineca.it

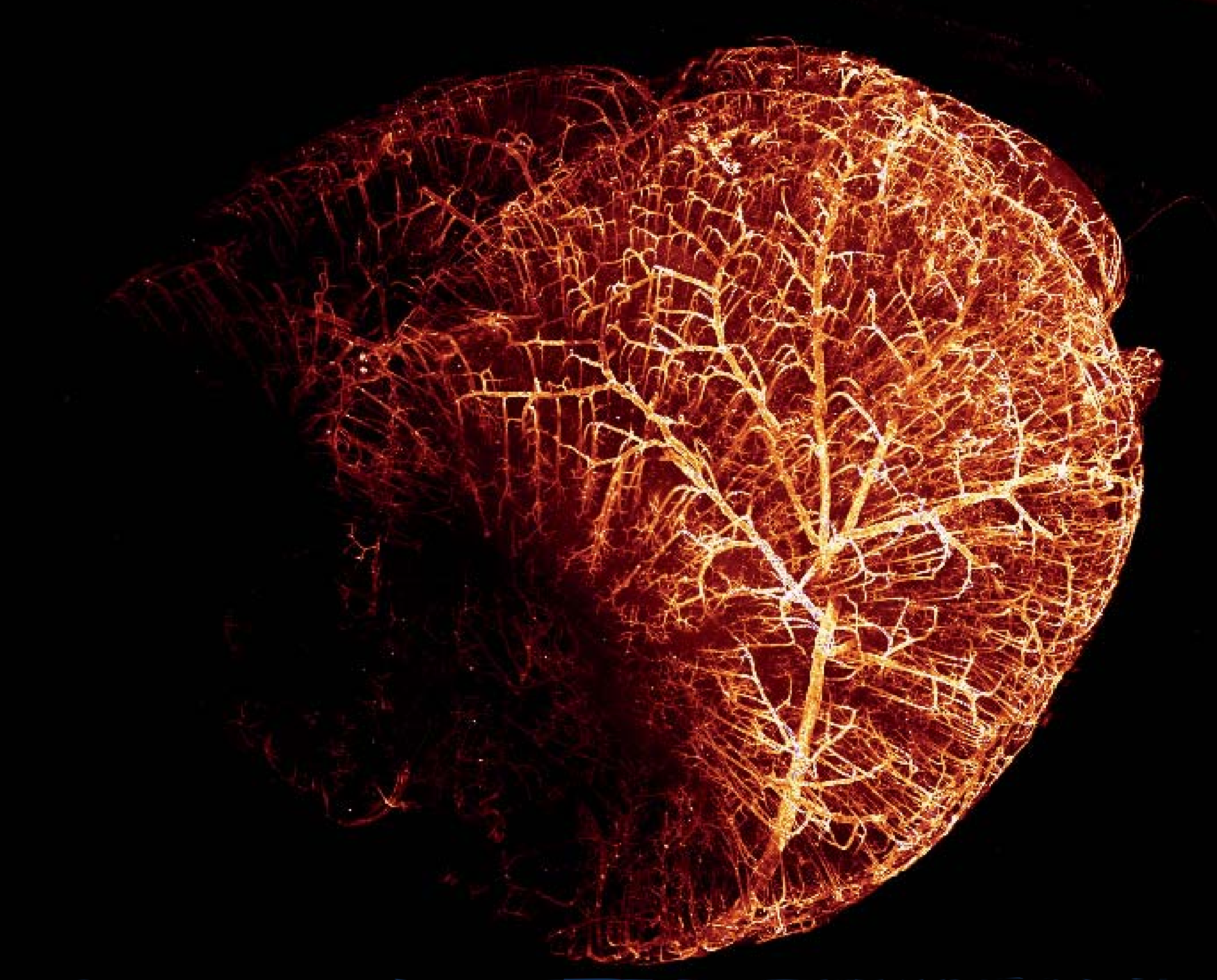


Figure 1: Laser scan of a mouse cerebellum portion. Courtesy of the European Laboratory for Non-Linear Spectroscopy, Florence, Italy

Figure 2: Where are research data commonly stored within your organization/laboratory?

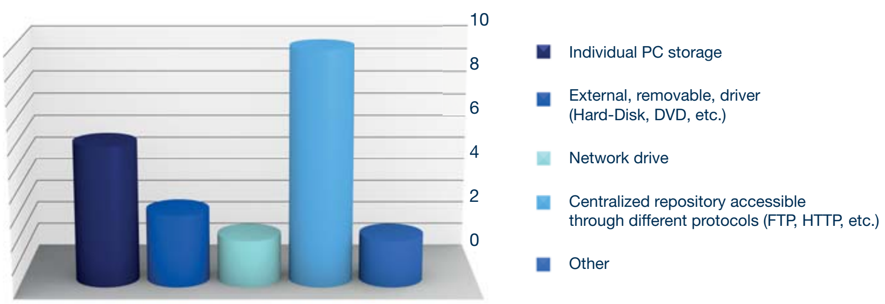
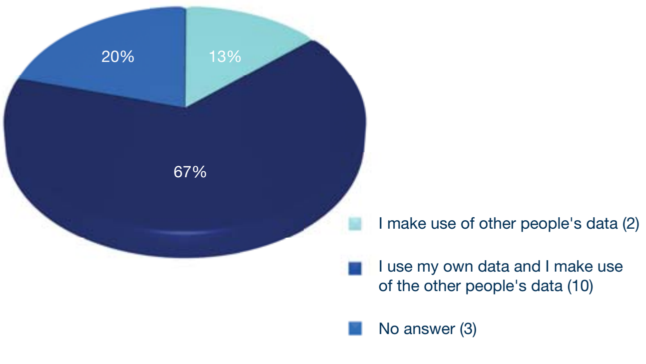


Figure 3: Do you use data generated by other scientists/groups?



Scientific Big Data

From assessment to implementation, Cineca offers high-level services designed specifically for users needs while maximizing return of effort investment and anticipating further growth.
Access to HPC resources is complemented with services for data curation and preservation, including remote visualization, computational workflow design and enhancement, resource consumption monitoring and metering.

Data curation and preservation
The enormous amount of data being produced on Cineca's HPC systems and the growing requests of Italian scientific communities to take care of their data sets, has led the SCAI department to design services for the curation of research data. Since the beginning of 2013, a data repository service has been available to those users who need to preserve their data in the medium-long term. The service has been designed to archive scientific data sets while providing mechanisms to easily manage and access them through a large variety of interfaces, including web browser, desktop client and command line tools. The service architecture has been carefully designed to scale to millions of files and petabytes of data, combining robustness and versatility, and to offer to the scientific communities a complete set of features to manage the whole data life-cycle. To achieve this the service provides the following functions: a) Upload/Download: the system supports high performance transfer protocols like GridFTP, or iRODS multi-threads transfer mechanism, and large interoperable ones like HTTP; b) Metadata management: each object can be associated to specific metadata represented as triplets (name,value,unit), or simply tagged and commented; c) Rules based management: common or per-project management rules can be specified to enforce/execute management policies; d) Stage-in/stage-out: the service is enabled to ship data sets towards HPC resources for being processed and backwards to ingest produced results.

Remote visualization
The possibility to remotely visualize data has become a fundamental requirement for those users who need to analyze and process huge data sets directly on the machine where they have been produced. Instead of transferring GBs of data and visualizing them on their personal computer - limited in memory and CPU - users can now utilize the Cineca remote visualization service
(http://www.hpc.cineca.it/services/remote-visualisation) to access their data and display them via low-cost hardware. The service leverages the VirtualGL technology to permit the rendering of OpenGL calls and includes a thin client for facilitating user interaction. The client offers a simple graphic interface (Remote Connection Manager) that allows user to easily create and manage remote displays on Cineca visualization facility.
The picture shows the remote rendering of a 1TB data set obtained through a Confocal Light-Sheet Microscopy (CLSM) technique on a mouse brain (1 cubic cm). The service will be included into the toolkit made available to Human Brain Project scientists.

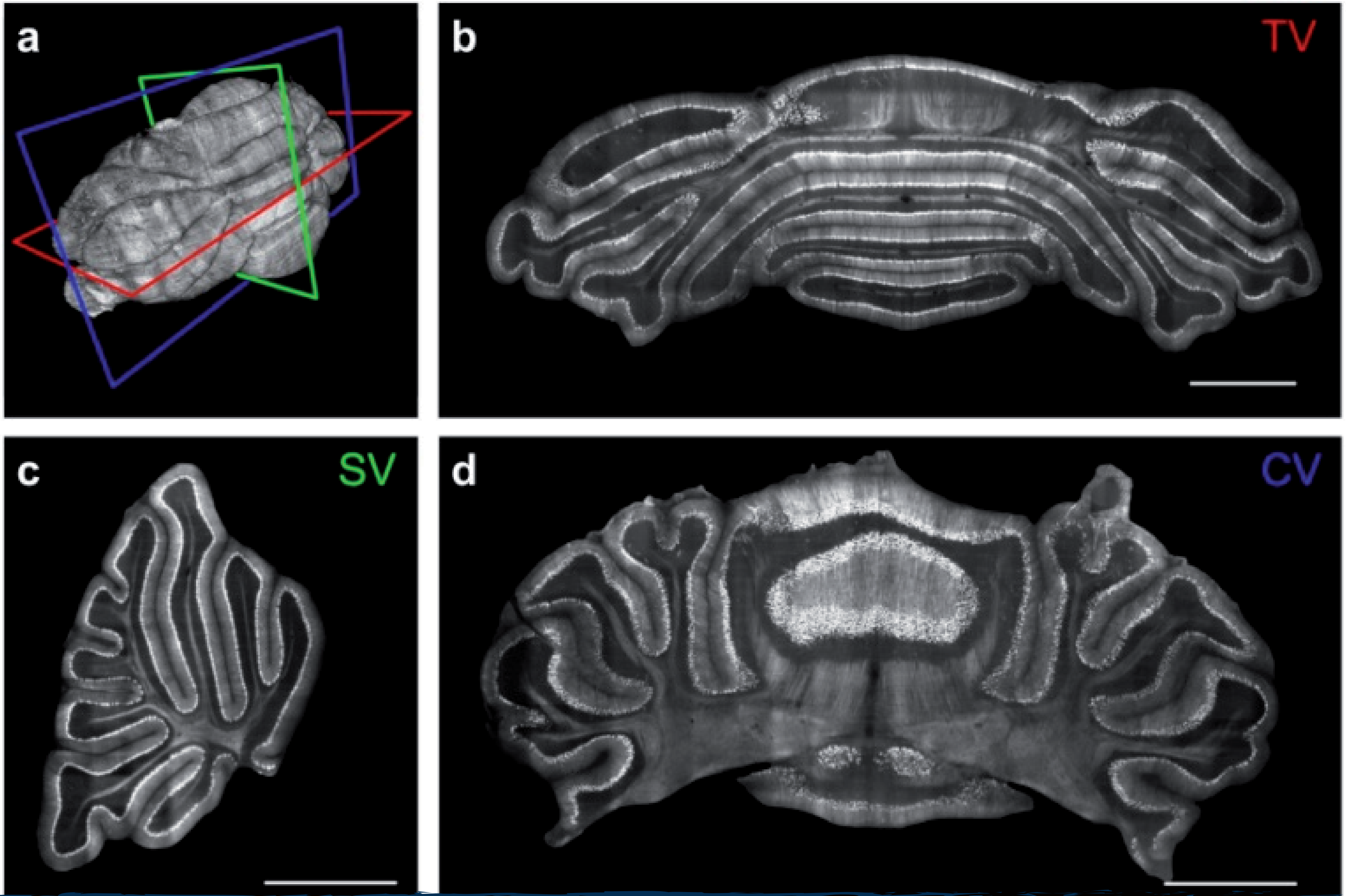


Figure 1: Laser scan of a mouse cerebellum portion. Courtesy of the European Laboratory for Non-Linear Spectroscopy, Florence, Italy

Cineca services are developed through the support and collaboration of different projects and initiatives in which the SCAI department is involved. The most relevant ones are listed below.

EUDAT (www.eudat.eu) - three-year project aiming at delivering a Collaborative Data Infrastructure (CDI) with the capacity and the capability to address cross-disciplinary requirements for proper data management and long-term preservation. Cineca represents one of the core nodes of the infrastructure and it is involved into the replication of seismic data sets collected by the Italian Institute of Seismology and Volcanology (INGV).

EUHIT (www.euhit.org) - project aiming at advancing the competitive edge of turbulence research in Europe. Cineca contributes with the resources and knowledge to implement the “Digital Library of Turbulence Data”, providing the Europe’s largest digital library service for data coming from numerical simulations and experiments in the field of Turbulence.

Research Data Alliance (www.rd-alliance.org) - initiative focusing at accelerating and facilitating research on data sharing and exchange at a global scale through promoting and encouraging bottom-up and interdisciplinary approach to solve these global challenges.

SoSIna (www.nextdataproject.it) - Italian project dealing with the retrieval, storage, access and sharing of environment and climate data from mountain and marine areas. During the project Cineca, in collaboration with the Italian National Research Council (CNR IIA), will develop a web portal to provide a homogeneous access to sparse thematic archives. The final interface will provide services like discovery, evaluation, access, and visualization, and will allow users to identify and access information from a wide range of local and global sources.

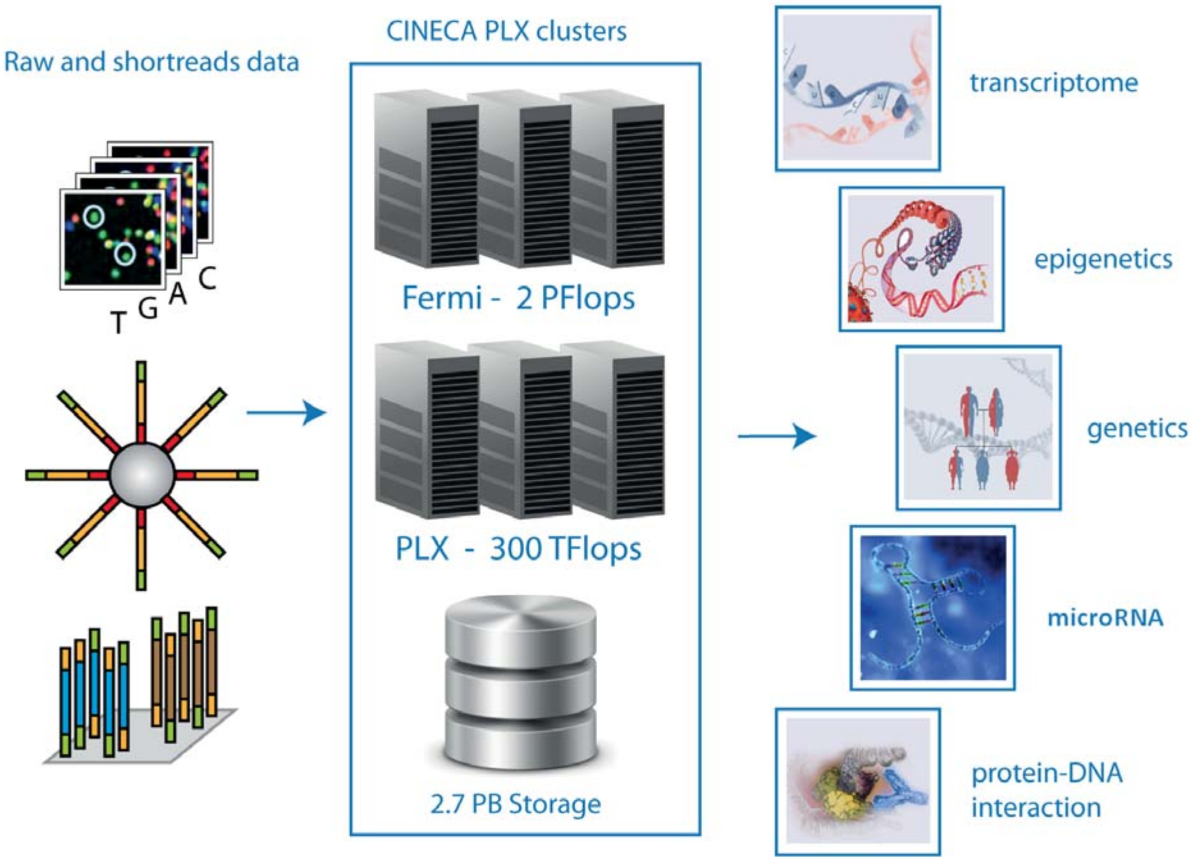
e-Health Applications

Next-generation DNA sequencing (NGS) has incredibly accelerated biological and biomedical research, by allowing the comprehensive analysis of genomes, transcriptomes and interactomes.
Managing the huge amount of data from new sequencing platforms requires non trivial skills, strong computational power and storage capacity which are generally not available in most research labs.
Cineca has been recognized as a big data center and HPC analysis for the Italian epigenomic flag project, Epigen.
The Cineca centralized bioinformatics core facility provides shared resources for the computational and IT requirements.
The exceptional Cineca hardware resources have been dedicated to this service both in terms of computational power and storage capacity.
The variety of available software that is continuously updated, and the long standing bioinformatics skills provide all research users an efficient, reliable and reproducible analysis of their short reads data.
The Cineca bioinformatics platform contains most of the current and emerging applications for NGS, such as new software tools and front-end methods for the selection of relevant genomic subsets.
The software system provided is able to perform analysis in the major applications of NGS:

- identification of DNA protein interactions by ChIP-seq;
- transcriptome profiling;
- miRNAs and other ncRNAs discovery;
- epigenetic analyses;
- SNVs detection;
- RNA Editing sites detection.

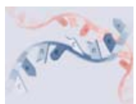
Web tools and databases have been developed for storing, rapidly assembling and analysing data generated from NGS platforms.
Key features of the facility include:

- cost-effective and easy access on thousands of computing cores;
- greatly increased speed and capacity for mapping algorithms;
- intuitive and flexible User Interface to accomodate most NGS projects.



Whole Exome Sequencing (WES) analysis is now available for several research purposes. A frequently updated pipeline is used to call variants, both SNPs and indels.
Variants are then filtered with many public databases including dbSNP, the 1000 Genomes project, HapMap exomes and more.
Variant prioritization is obtained by comparing disease and healthy controls and performing their functional annotation (e.g. the functional relevance of a protein variant is assessed by SITF software).
Moreover, for family-based samples, the advanced analysis of haplotype phasing and complex heterozygous or homologous mutations detection is available as well.

RNA-Seq (Transcriptome) analysis is now avaliable for transcriptome structural analysis and quantification. The transcriptome analysis allows the identification of known or novel expressed transcript variants, and their quantification.
RNA-Seq, unlike microarrays, does not require prior knowledge of the genome and therefore offers several advantages. Our facility can study the transcriptome profiling of each sample, performs differential gene expression analysis, cassette exons, chimeric transcripts and polyA sites detection.
ChIP-Seq is widely used to analyze DNA-protein interactions. It combines chromatin immunoprecipitation (ChIP) with massively parallel DNA sequencing to identify binding sites of DNA-associated proteins, and can be used to precisely map global binding sites for any protein of interest. Our bioinformatic service provides Genome-wide distribution of ChIP sequencing reads, peak identification and differential analysis across different samples.



RNA editing is a widespread post-transcriptional molecular phenomenon that can increase proteomic diversity. In order to detect editing sites supported by data obtained by RNA-Seq experiments the ExpEdit pipeline carries out carry out a comparative analysis against a large collection of known editing sites collected in DARNED database as well as other user-provided potentially edited positions.5. NGS Data Repository
A big data management system can provide extra data-mining features to federate data derived from several NGS experiments. In order to adapt to the much greater input and output demand of bioinformatics data analyses, the NGS Data Repository (NGSDR) incorporates some up-to-date technological improvements:
- the separation of input metadata from the content, based on iRODS (Integrated Rule-Oriented Data System) technology;
- a seamless interaction between metadata structural information, alignments, input, and stored results data, thanks to the most recent web design and content standards.
- Inter-databases relationships allowing search and links to NCBI databases, UCSC genome browser's annotations and other secondary repositories.
- simple submission procedures supporting standard data formats (fasta, fastq, BAM, SAM, gzip, tar.gz) from the NGS research community.
- In addition to archiving and querying data, tutorials, filtering forms and tooltips are provided to assist CINECA users of all levels of expertise to quickly find, analyze, visualize and download NGS data.
In NGSDR an experiment can be submitted uploading the short reads files and specifying metadata information according to the EBI/ENA Sequence Read Archive (SRA) data format standards (www.ebi.ac.uk/ena/about/sra_format).

The Impact of Cineca HPC Infrastructure on the Research Community

The HPC infrastructure of Cineca is open to national and international researchers and research organizations needing large allocations of computer time to address big challenges in science and engineering. Through the peer-review based programmes PRACE, ISCRA and LISA, Cineca supports its mission of offering the best available infrastructure acting as national HPC facility.

After 5 years of implementation of such initiatives, the need of discovering the relative importance of Cineca on the Italian researchers' career and also evaluating the return of investment clearly emerged; we decided to analyze the impact that our services had on the national scientific communities and on innovation at large, with the aim of continuously improving and tailoring the range of services offered.

The analysis is focused on the publications and citations of the Italian researchers using HPC in all the science and engineering fields, as well as on some other European terms of comparison, using Web of Knowledge as the reference database and on the basis of a five years timespan (2008-2013).

470 publications by Italian PIs mentioned Cineca as the main funding agency for the project, a subset of these has also some co-funding agencies, mostly the European Commission (13,3%), INAF National Institute for Astrophysics (10%) and Caspur (8,3%). The research areas of major weight in the total number are Physics (50,6%), Chemistry (37,1%), Material science (11,0%) and Astrophysics (10,8%) (each publication can belong to multiple areas). A number of these highlights international collaborations in the research teams, 11% with USA, 10% with France and Germany and 8% with Spain.

Querying the citations for the same "Cineca" string, a total of 2.545 citations is registered, with an average citations number per item of 5,4.

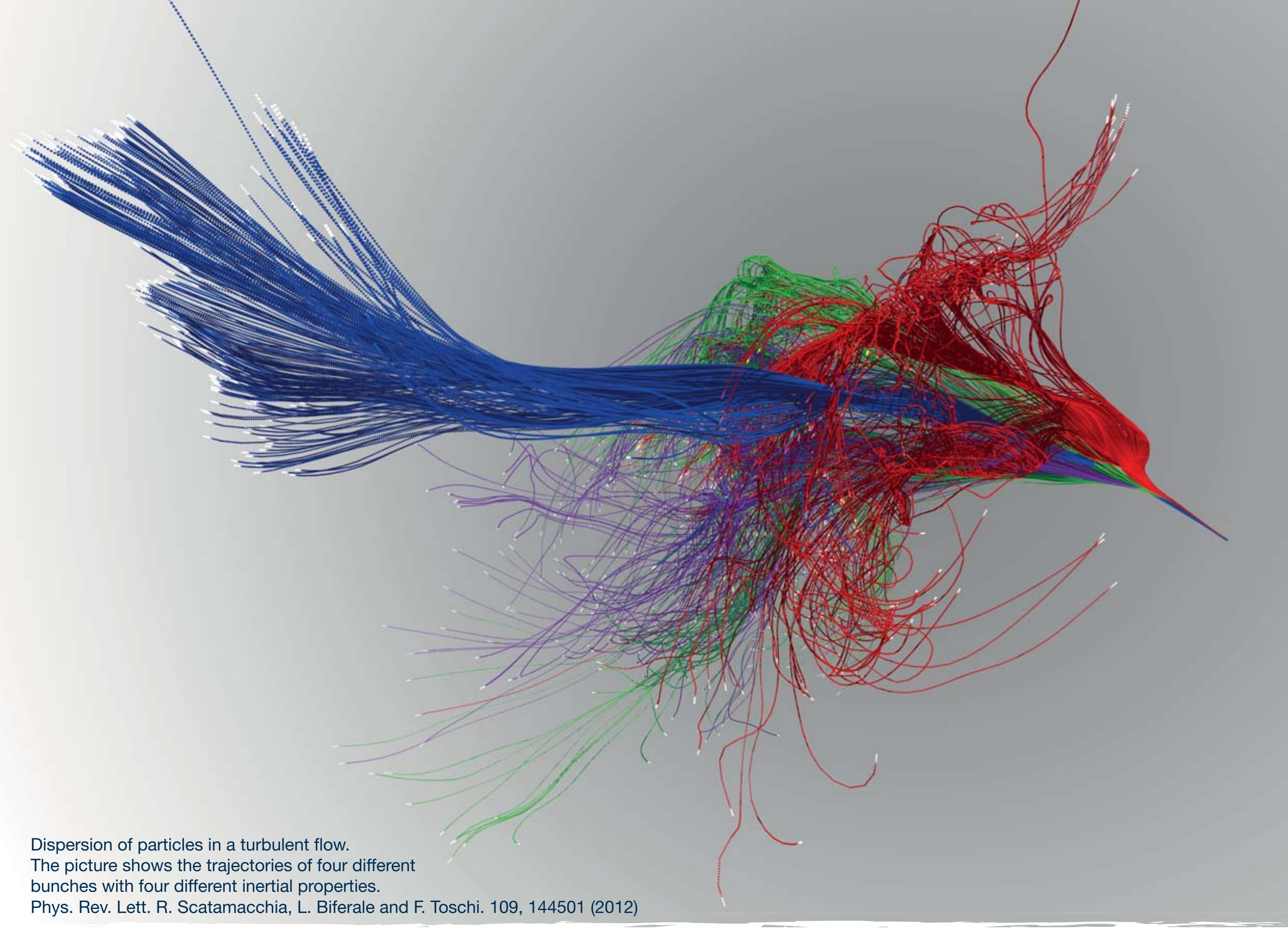
The most cited article results to be "Yambo: An ab initio tool for excited state calculations", 2009, by Marini, Hogan, Gruening, and Varsano, with the very high number of 115 citations.

The same percentages of research fields and international collaborations appear querying "ISCRA" as funding agency, for a total of 135 publication, an outstanding result considering that the first ISCRA calls were issued in 2010 and the first round of projects closed in early 2011.

A comparison with the other PRACE Tier 0 sites or countries, depending on the cases, (e.g. FZJ with some 520 publications, GENCI with 685 - including three French sites, …) applying the same research criteria used for Cineca, clearly demonstrates that Italy maintains its position in the field of the European players.

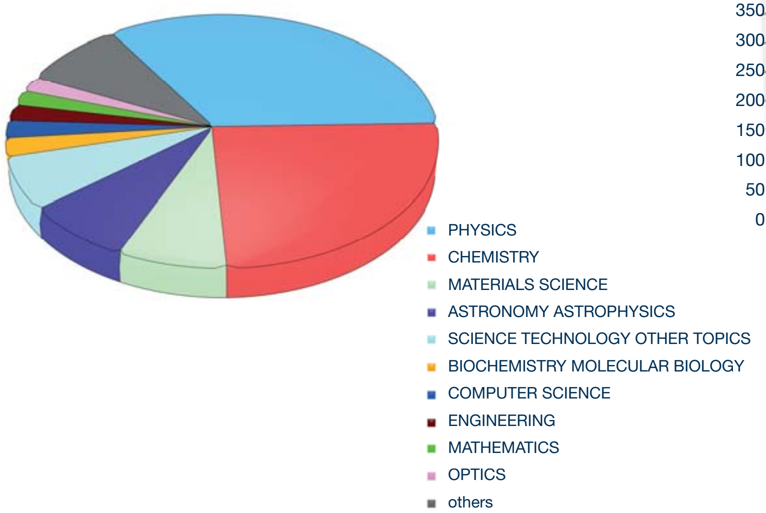
Further, the data demonstrate two relevant conclusions. One is a significantly growing tendency in the number of publications based on usage of Cineca resources; the increasing trend line of the number of publications and citations over time confirms that the services offered by Cineca allow the national research to remain competitive in a very challenging environment characterized by an extremely rapid technological innovation. The other is the growing collaborations (co-PIs) among Cineca and the most relevant Italian research institutes, like INFN, CNR, SISSA-ISAS, OGS, INGV, that confirms and reinforces the position of Cineca as the high performance computing national infrastructure, providing, besides highly specialized technical consultancy, huge (even if never sufficient, given the exponentially growing demand) amounts of computing time and cutting-edge data solutions.

(The whole report is available on www.hpc.cineca.it)



Dispersion of particles in a turbulent flow.
The picture shows the trajectories of four different bunches with four different inertial properties.
Phys. Rev. Lett. R. Scatamacchia, L. Biferale and F. Toschi. 109, 144501 (2012)

Figure 1: Research Areas of 472 publications by Italian PI that mentioned Cineca as the main funding agency for the project (each publication can belong to multiple areas)



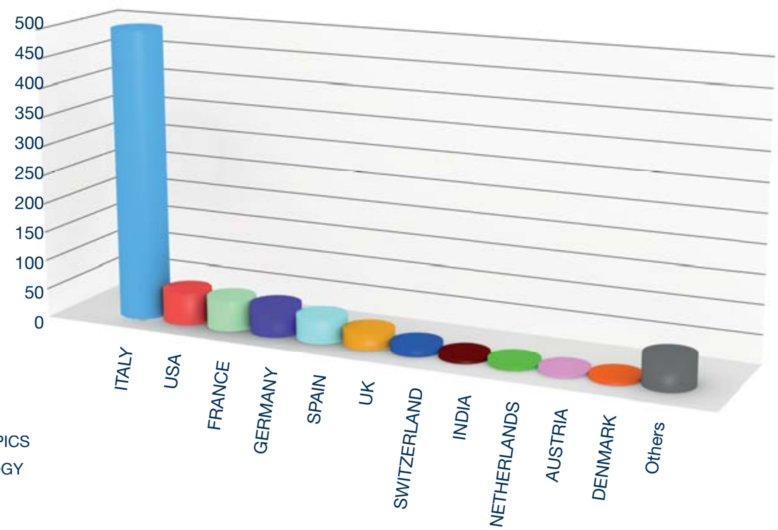
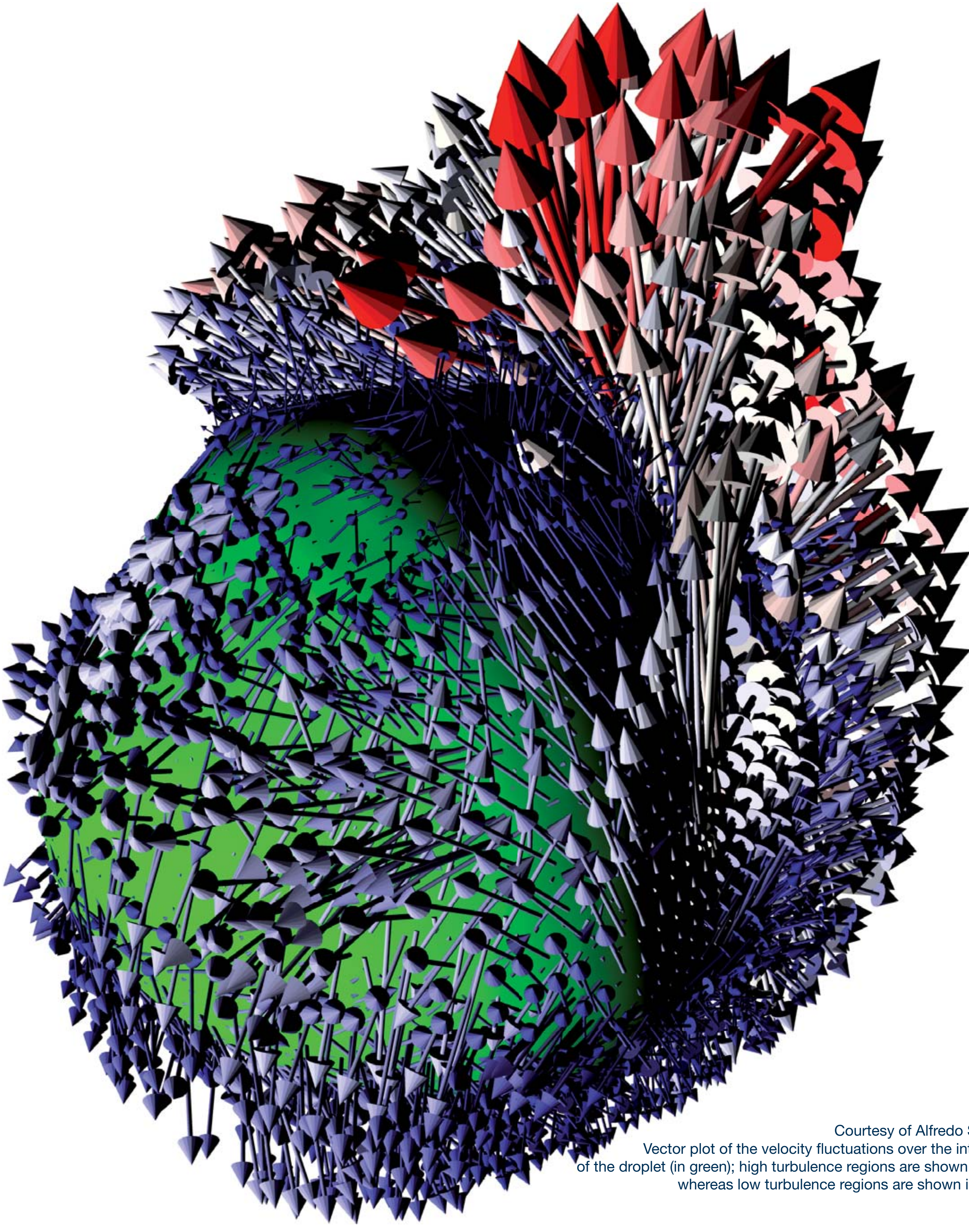


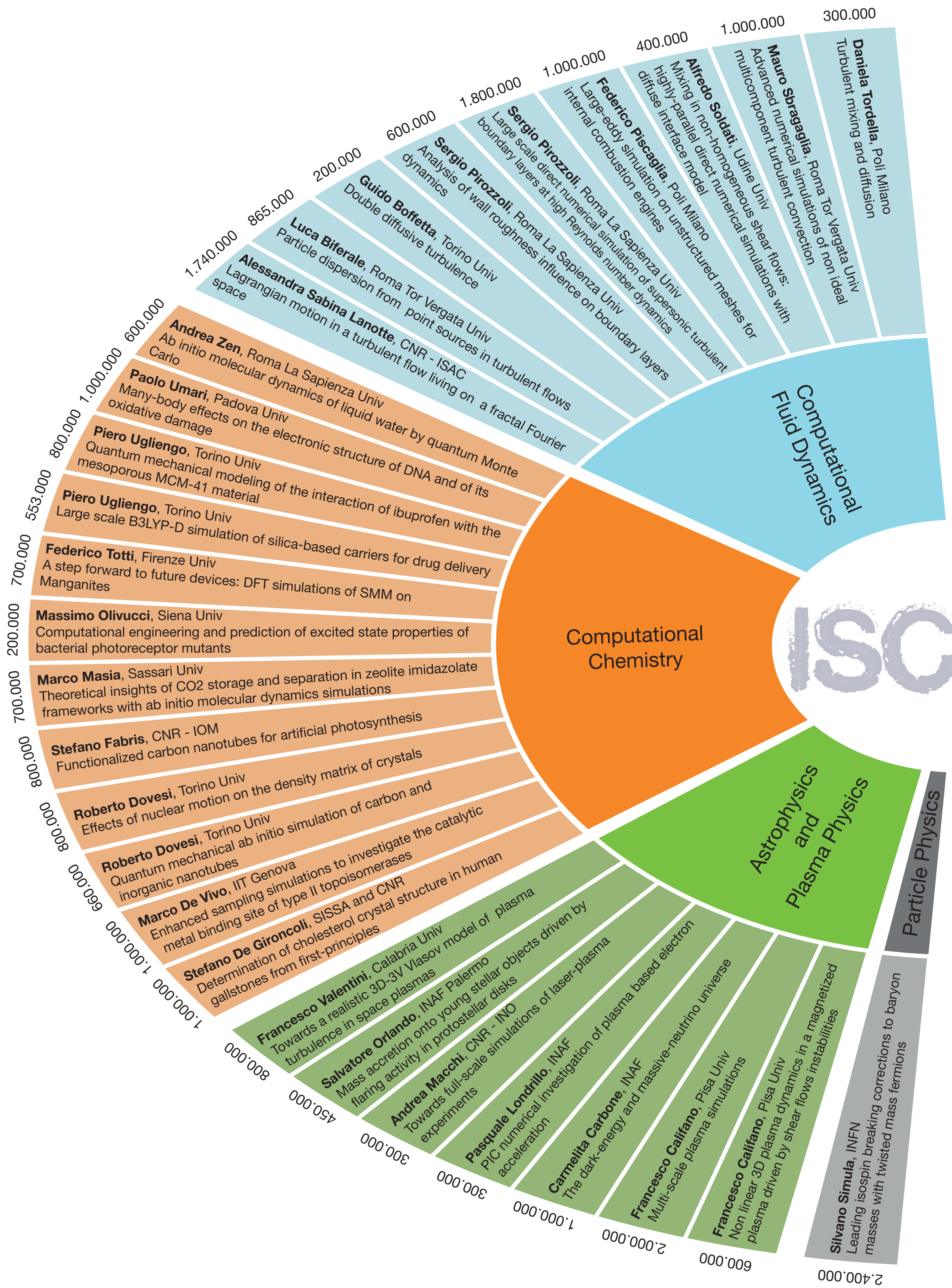
Figure 2: International collaboration in the research teams with Italian PI

Presentation of the Users' Reports

In summer 2012 and at the very beginning of 2013, the installation of the new HPC systems, Fermi and Eurora, represented an amazing boost of resources available at national and European level.
In addition to the existing and still in production system, PLX, the two new machines enabled the Cineca supercomputing infrastructure to deliver more than 1 billion of core-hours per year.
Since the entry into production of the current systems configuration, a total of 1877 projects were activated for a global amount of more than 3200 active users on the systems, that presented an average load around 80% with peaks near 90%.
The projects are activated according to the specific allocation channel, PRACE, ISCRA, LISA or, as a residual margin, as development projects and as projects related to agreements of joint collaboration between Cineca and outstanding national research entities.
One of the missions of SCAI is enabling researchers to attack the scientific challenges of their domain, focusing only on science and benefiting, for all HPC matters, from the extensive experience and specialized skills of the SCAI technical staff. A very powerful support to researchers who request that, is offered by the *in-loco* 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.
The following pages contain a selection (made on the basis of the availability of the data at the time of this publication) of the reports that are required to each Principal Investigator, in order to share and disseminate the results of the research project. The reports (some included in full, others only as abstracts) refer to users selected via ISCRA and LISA at the national level, and through PRACE at the European level.
Regarding the PRACE projects, the charts offer a complete overview of all the Italian PIs who obtained an award on any of the PRACE Tier 0 systems, as well as a picture of all the PIs, Italian and worldwide, who have received an award through PRACE on FERMI at Cineca.

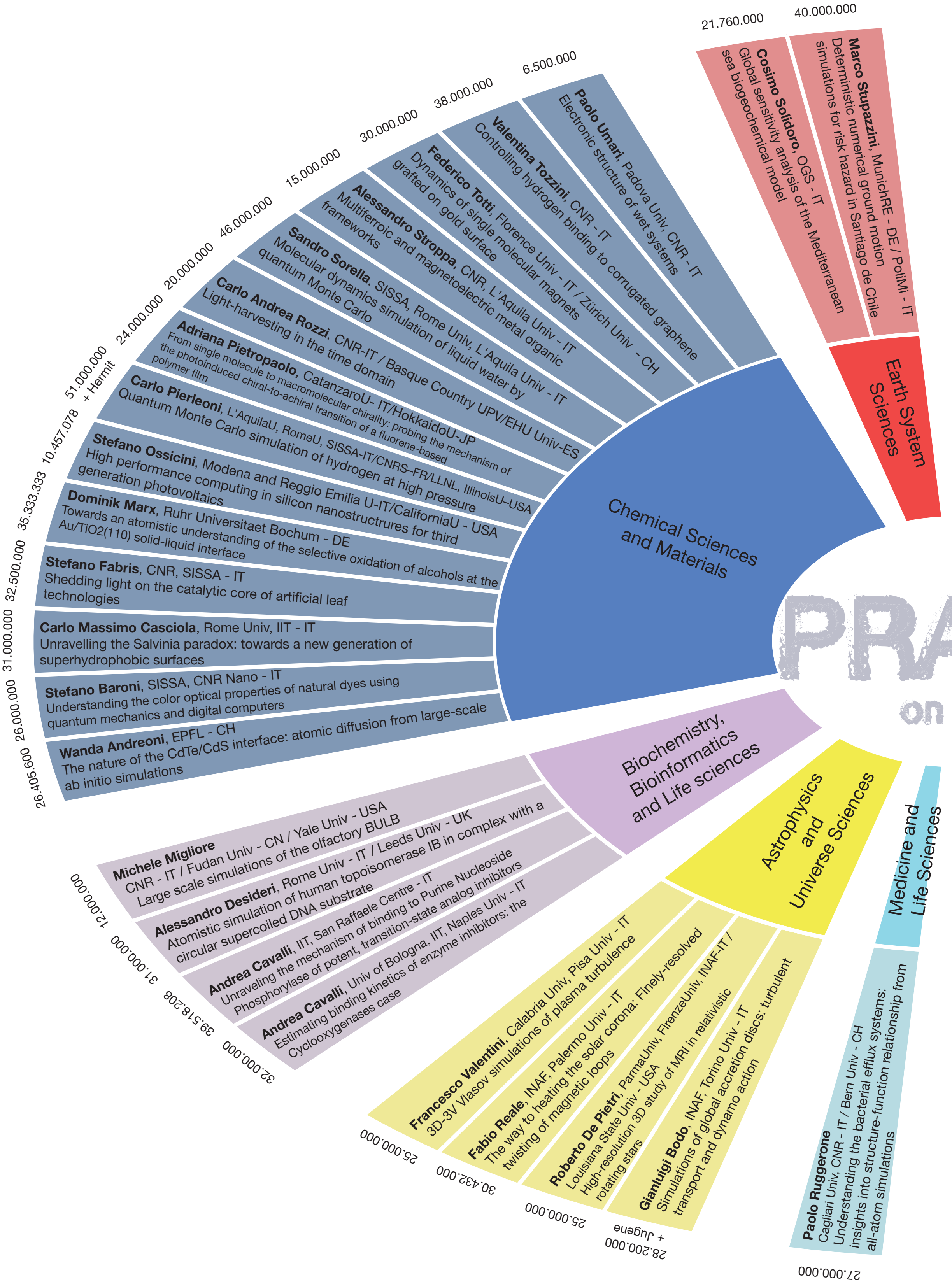


Courtesy of Alfredo Soldati
Vector plot of the velocity fluctuations over the interface of the droplet (in green); high turbulence regions are shown in red, whereas low turbulence regions are shown in blue.



ISC
Computational Fluid Dynamics
Daniela Tordella, Poli Milano
Turbulent mixing and diffusion
300.000
Mauro Sbragaglia, Roma Tor Vergata Univ
Advanced numerical simulations of non ideal multicomponent turbulent convection
1.000.000
Alfredo Soldati, Udine Univ
Mixing in non-homogeneous shear flows: highly-parallel direct numerical simulations with diffuse interface model
400.000
Federico Piscaglia, Poli Milano
Large-eddy simulation on unstructured meshes for internal combustion engines
1.000.000
Sergio Pirozzoli, Roma La Sapienza Univ
Large scale direct numerical simulation of supersonic turbulent boundary layers at high Reynolds number dynamics
1.800.000
Sergio Pirozzoli, Roma La Sapienza Univ
Analysis of wall roughness influence on boundary layers dynamics
600.000
Guido Boffetta, Torino Univ
Double diffusive turbulence
200.000
Luca Biferale, Roma Tor Vergata Univ
Particle dispersion from point sources in turbulent flows
865.000
Alessandra Sabina Lanotte, CNR - ISAC
Lagrangian motion in a turbulent flow living on a fractal Fourier space
1.740.000
Computational Chemistry
Andrea Zen, Roma La Sapienza Univ
Ab initio molecular dynamics of liquid water by quantum Monte Carlo
600.000
Paolo Umari, Padova Univ
Many-body effects on the electronic structure of DNA and of its oxidative damage
1.000.000
Piero Ugliengo, Torino Univ
Quantum mechanical modeling of the interaction of ibuprofen with the mesoporous MCM-41 material
800.000
Piero Ugliengo, Torino Univ
Large scale B3LYP-D simulation of silica-based carriers for drug delivery
553.000
Federico Totti, Firenze Univ
A step forward to future devices: DFT simulations of SMM on Manganites
700.000
Massimo Olivucci, Siena Univ
Computational engineering and prediction of excited state properties of bacterial photoreceptor mutants
200.000
Marco Masia, Sassari Univ
Theoretical insights of CO2 storage and separation in zeolite imidazolate frameworks with ab initio molecular dynamics simulations
700.000
Stefano Fabris, CNR - IOM
Functionalized carbon nanotubes for artificial photosynthesis
800.000
Roberto Dovesi, Torino Univ
Effects of nuclear motion on the density matrix of crystals
800.000
Roberto Dovesi, Torino Univ
Quantum mechanical ab initio simulation of carbon and inorganic nanotubes
660.000
Marco De Vivo, IIT Genova
Enhanced sampling simulations to investigate the catalytic metal binding site of type II topoisomerases
1.000.000
Stefano De Gironcoli, SISSA and CNR
Determination of cholesterol crystal structure in human gallstones from first-principles
1.000.000
Astrophysics and Plasma Physics
Francesco Valentini, Calabria Univ
Towards a realistic 3D-3V Vlasov model of plasma turbulence in space plasmas
800.000
Salvatore Orlando, INAF Palermo
Mass accretion onto young stellar objects driven by flaring activity in protostellar disks
450.000
Andrea Macchi, CNR - INO
Towards full-scale simulations of laser-plasma experiments
300.000
Pasquale Londrillo, INAF
PIC numerical investigation of plasma based electron acceleration
300.000
Carmelita Carbone, INAF
The dark-energy and massive-neutrino universe
1.000.000
Francesco Califano, Pisa Univ
Multi-scale plasma simulations
2.000.000
Francesco Califano, Pisa Univ
Non linear 3D plasma dynamics in a magnetized plasma driven by shear flows instabilities
600.000
Particle Physics
Silvano Simula, INFN
Leading isospin breaking corrections to baryon masses with twisted mass fermions
2.400.000

Condensed Matter Physics
Earth and Climate Science
Bioinformatics
Computational biology
900.000
Marco Bernasconi, Milano Bicocca Univ
Simulation of GeTe nanowires for phase change memories
350.000
Ezio Bruno, Messina Univ
Ab initio study of phase transitions in metallic alloys: equilibrium thermodynamics and kinetics
900.000
Giovanni Cantele, CNR - SPIN
Optical response, excitons and electronic correlations in TiO2 nanomaterials: novel insights from a fully ab-initio many-body perturbation theory approach
4.600.000
Stefano De Gironcoli, SISSA and CNR - IOM
Benchmark calculations in molecular systems with self-consistent-field EXX RPA functional
800.000
Francesco Filippone, CNR - ISM
Properties of interfaces in ternary hybrid materials for photovoltaic applications
450.000
Alessandro Laio, SISSA
Simulation of fibril nuceation process of the C-terminal domain of A-beta protein
1.600.000
Ivan Marri, Modena and Reggio Emilia Univ
Multiexcitons at a cost of one: carrier multiplication in silicon nanocrystals
640.000
Carlo Pierleoni, L'Aquila Univ
Coupled electron-ion Monte Carlo study of high pressure hydrogen
1.800.000
Maria Clelia Righi, Modena and Reggio Univ, CNR - NANO
Understanding boundary lubrication. The case of mechanically-induced surface modifications in carbon interfaces
1.200.000
Paolo Ruggerone, Cagliari Univ
Efflux systems and bacterial resistance: computer simulations facing an emergence
560.000
Silvano Simula, INFN
A new approach to b-physics on current lattices
600.000
Sandro Sorella, SISSA
Magnetism and high temperature superconductivity in pnictides
1.900.000
Alessandro Stroppa, CNR - SPIN
Ab-initio study of new multiferroic metal-organic frameworks (MOFs)
3.200.000
Federica Magnoni, INGV
Spectral-element and adjoint 3D full-wave tomography for Italy
933.890
Stefano Salon, OGS
Multi-decadal simulations of the Mediterranean sea biogeochemical cycles
400.000
Gianmaria Sannino, ENEA
Evaluating the effects produced by tides on mthc
1.400.000
Sergio Mauro Solinas, Pavia Univ
Realistic computational modeling of the cerebellum
600.000
Andrea Benazzo, Ferrara Univ
Temporal sampling scheme and demographic inferences in population genetics
960.000
Giovanni Bussi, SISSA
RNA-protein binding by means of massively-parallel biased simulations
455.000
Rosa Di Felice, CNR - NANO
Simulating protein unfolding under pulling force
200.000
Francesca Fanelli, Modena and Reggio Emilia Univ
High-throughput virtual screening of inhibitors of RhoA-Lbc interaction
200.000
Alfonso Gautieri, Poli Milano
Molecular dynamics based investigation of microscale and mesoscale mechanisms of osteogenesis imperfecta
819.200
Alessandro Laio, SISSA
Simulation of polypeptide aggregation in explicit solvent by bias-exchange metadynamics
220.000
Alessandra Magistrato, CNR - IOM
The inward-to-outward conformational change in the transport mechanism of sodium-coupled galactose symporter investigated by bias exchange metadynamics simulations
2.002.000
Alessandra Magistrato, CNR - IOM
The inward-to-outward conformational change relying on the transport mechanism of sodium-coupled galactose symporter investigated by bias exchange metadynamics simulations
4.800.000
Simone Melchionna, CNR - IAC
Resistance of thermostable proteins to flow conditions
3.000.000
Adriana Pietropaolo, Catanzaro Univ
Environment effects on the efficiency of open-closure enzyme mediated mechanisms
200.000
Giulio Rastelli, Modena and Reggio Emilia Univ
Binding estimation after refinement, a powerful tool for virtual screening of potential drugs
500.000
Attilio Vittorio Vargiu, CNR - IOM
Addressing resistance mechanisms in Gram-negative bacteria: molecular modeling of influx and efflux of antibiotics
733.000
Attilio Vittorio Vargiu, CNR - IOM
Molecular description of efflux dynamics in Gram-negative bacteria: an extensive study on antibiotics and inhibitors of E.coli and P.Aeruginosa RND pumps
872.450



Earth System Sciences
21.760.000
Cosimo Solidoro, OGS - IT
Global sensitivity analysis of the Mediterranean sea biogeochemical model
40.000.000
Marco Stupazzini, MunichRE - DE / PoliMi - IT
Deterministic numerical ground motion simulations for risk hazard in Santiago de Chile
Chemical Sciences and Materials
6.500.000
Paolo Umari, Padova Univ, CNR - IT
Electronic structure of wet systems
38.000.000
Valentina Tozzini, CNR - IT
Controlling hydrogen binding to corrugated graphene
30.000.000
Federico Totti, Florence Univ - IT / Zürich Univ - CH
Dynamics of single molecular magnets grafted on gold surface
15.000.000
Alessandro Stroppa, CNR, L'Aquila Univ - IT
Multiferroic and magnetoelectric metal organic frameworks
46.000.000
Sandro Sorella, SISSA, Rome Univ, L'Aquila Univ - IT
Molecular dynamics simulation of liquid water by quantum Monte Carlo
20.000.000
Carlo Andrea Rozzi, CNR-IT / Basque Country UPV/EHU Univ-ES
Light-harvesting in the time domain
24.000.000
Adriana Pietropaolo, CatanzaroU- IT/HokkaidoU-JP
From single molecule to macromolecular chirality: probing the mechanism of the photoinduced chiral-to-achiral transition of a fluorene-based polymer film
51.000.000
+ Hermit
Carlo Pierleoni, L'AquilaU, RomeU, SISSA-IT/CNRS–FR/LLNL, IllinoisU–USA
Quantum Monte Carlo simulation of hydrogen at high pressure
10.457.078
Stefano Ossicini, Modena and Reggio Emilia U-IT/CaliforniaU - USA
High performance computing in silicon nanostructrures for third generation photovoltaics
35.333.333
Dominik Marx, Ruhr Universitaet Bochum - DE
Towards an atomistic understanding of the selective oxidation of alcohols at the Au/TiO2(110) solid-liquid interface
32.500.000
Stefano Fabris, CNR, SISSA - IT
Shedding light on the catalytic core of artificial leaf technologies
31.000.000
Carlo Massimo Casciola, Rome Univ, IIT - IT
Unravelling the Salvinia paradox: towards a new generation of superhydrophobic surfaces
26.000.000
Stefano Baroni, SISSA, CNR Nano - IT
Understanding the color optical properties of natural dyes using quantum mechanics and digital computers
26.405.600
Wanda Andreoni, EPFL - CH
The nature of the CdTe/CdS interface: atomic diffusion from large-scale ab initio simulations
Biochemistry, Bioinformatics and Life sciences
12.000.000
Michele Migliore
CNR - IT / Fudan Univ - CN / Yale Univ - USA
Large scale simulations of the olfactory BULB
31.000.000
Alessandro Desideri, Rome Univ - IT / Leeds Univ - UK
Atomistic simulation of human topoisomerase IB in complex with a circular supercoiled DNA substrate
39.518.208
Andrea Cavalli, IIT, San Raffaele Centre - IT
Unraveling the mechanism of binding to Purine Nucleoside Phosphorylase of potent, transition-state analog inhibitors
32.000.000
Andrea Cavalli, Univ of Bologna, IIT, Naples Univ - IT
Estimating binding kinetics of enzyme inhibitors: the Cyclooxygenases case
Astrophysics and Universe Sciences
25.000.000
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3D-3V Vlasov simulations of plasma turbulence
30.432.000
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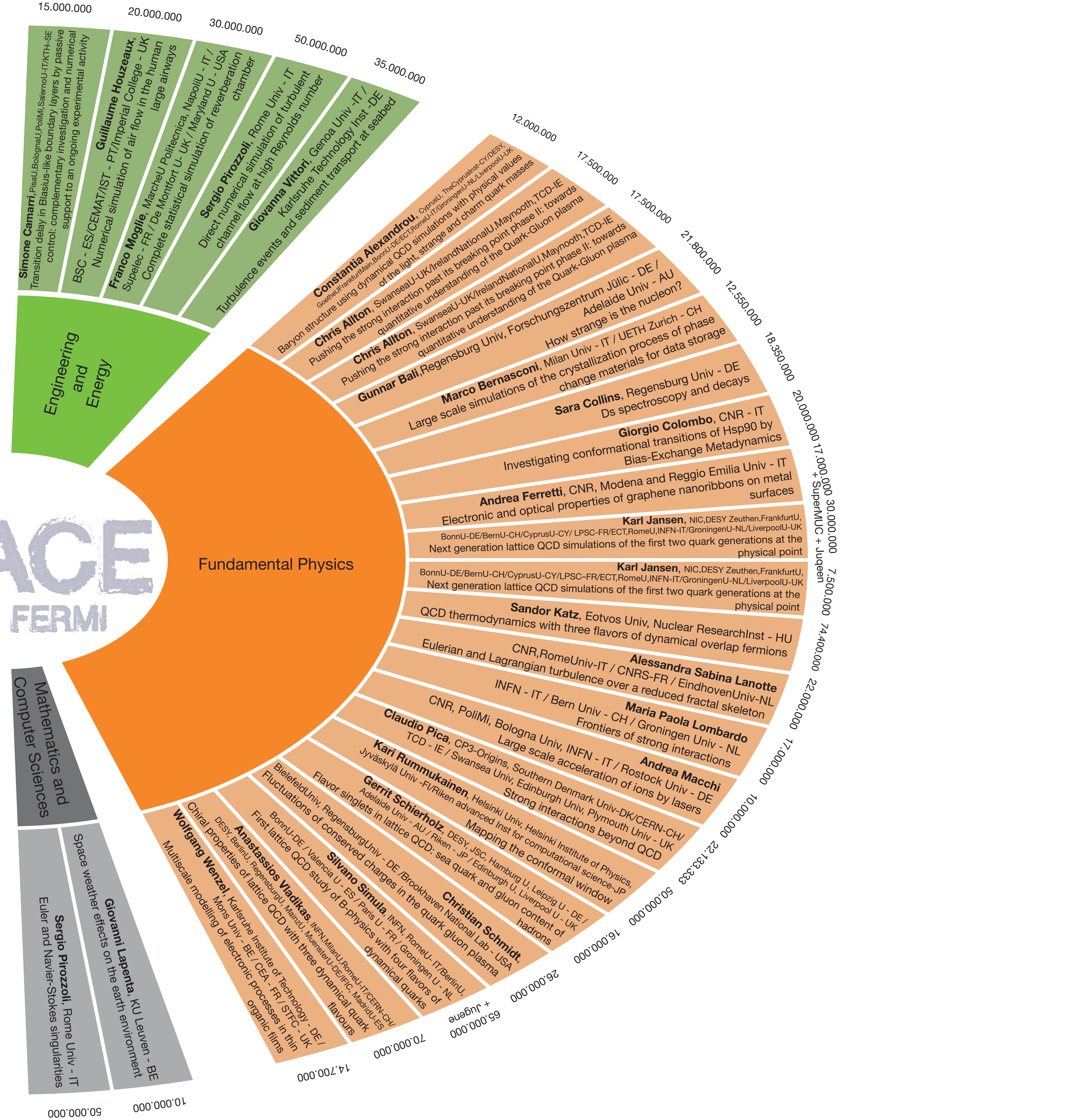
The way to heating the solar corona: Finely-resolved twisting of magnetic loops
25.000.000
Roberto De Pietri, ParmaUniv, FirenzeUniv, INAF-IT / Louisiana State Univ - USA
High-resolution 3D study of MRI in relativistic rotating stars
28.200.000
+ Jugene
Gianluigi Bodo, INAF Torino Univ - IT
Simulations of global accretion discs: turbulent transport and dynamo action
Medicine and Life Sciences
27.000.000
Paolo Ruggerone
Cagliari Univ, CNR - IT / Bern Univ - CH
Understanding the bacterial efflux systems: insights into structure-function relationship from all-atom simulations
PRA
on



Engineering and Energy
Fundamental Physics
Mathematics and Computer Sciences
FERMI
Simone Camarri, PisaU,BolognaU,PoliMi,SalernoU-IT/KTH-SE
Transition delay in Blasius-like boundary layers by passive control: complementary investigation and numerical support to an ongoing experimental activity
15.000.000
Guillaume Houzeaux, BSC - ES/CEMAT/IST - PT/Imperial College - UK
Numerical simulation of air flow in the human large airways
20.000.000
Franco Moglie, MarcheU Politecnica, NapoliU - IT / Supelec - FR / De Montfort U- UK / Maryland U - USA
Complete statistical simulation of reverberation chamber
30.000.000
Sergio Pirozzoli, Rome Univ - IT
Direct numerical simulation of turbulent channel flow at high Reynolds number
50.000.000
Giovanna Vittori, Genoa Univ -IT / Karlsruhe Technology Inst -DE
Turbulence events and sediment transport at seabed
35.000.000
Constantia Alexandrou, CyprusU, TheCyprusInst-CY/DESY, GoetheUFrankfurtMain,BonnU-DE/ECT,RomeU-IT/GroningenU-NL/LiverpoolU-UK
Baryon structure using dynamical QCD simulations with physical values of the light, strange and charm quark masses
12.000.000
Chris Allton, SwanseaU-UK/IrelandNationalU,Maynooth,TCD-IE
Pushing the strong interaction past its breaking point phase II: towards quantitative understanding of the Quark-Gluon plasma
17.500.000
Chris Allton, SwanseaU-UK/IrelandNationalU,Maynooth,TCD-IE
Pushing the strong interaction past its breaking point phase II: towards quantitative understanding of the Quark-Gluon plasma
17.500.000
Gunnar Bali,Regensburg Univ, Forschungszentrum Jülic - DE / Adelaide Univ - AU
How strange is the nucleon?
21.800.000
Marco Bernasconi, Milan Univ - IT / UETH Zurich - CH
Large scale simulations of the crystallization process of phase change materials for data storage
12.550.000
Sara Collins, Regensburg Univ - DE
Ds spectroscopy and decays
18.350.000
Giorgio Colombo, CNR - IT
Investigating conformational transitions of Hsp90 by Bias-Exchange Metadynamics
20.000.000
Andrea Ferretti, CNR, Modena and Reggio Emilia Univ - IT
Electronic and optical properties of graphene nanoribbons on metal surfaces
17.000.000 + SuperMUC + Juqeen
Karl Jansen, NIC,DESY Zeuthen,FrankfurtU, BonnU-DE/BernU-CH/CyprusU-CY/ LPSC-FR/ECT,RomeU,INFN-IT/GroningenU-NL/LiverpoolU-UK
Next generation lattice QCD simulations of the first two quark generations at the physical point
30.000.000
Karl Jansen, NIC,DESY Zeuthen,FrankfurtU, BonnU-DE/BernU-CH/CyprusU-CY/LPSC–FR/ECT,RomeU,INFN-IT/GroningenU-NL/LiverpoolU-UK
Next generation lattice QCD simulations of the first two quark generations at the physical point
7.500.000
Sandor Katz, Eotvos Univ, Nuclear ResearchInst - HU
QCD thermodynamics with three flavors of dynamical overlap fermions
74.400.000
Alessandra Sabina Lanotte, CNR,RomeUniv-IT / CNRS-FR / EindhovenUniv-NL
Eulerian and Lagrangian turbulence over a reduced fractal skeleton
22.000.000
Maria Paola Lombardo, INFN - IT / Bern Univ - CH / Groningen Univ - NL
Frontiers of strong interactions
17.000.000
Andrea Macchi, CNR, PoliMi, Bologna Univ, INFN - IT / Rostock Univ - DE
Large scale acceleration of ions by lasers
10.000.000
Claudio Pica, CP3-Origins, Southern Denmark Univ-DK/CERN-CH/ TCD - IE / Swansea Univ, Edinburgh Univ, Plymouth Univ - UK
Strong interactions beyond QCD
22.133.333
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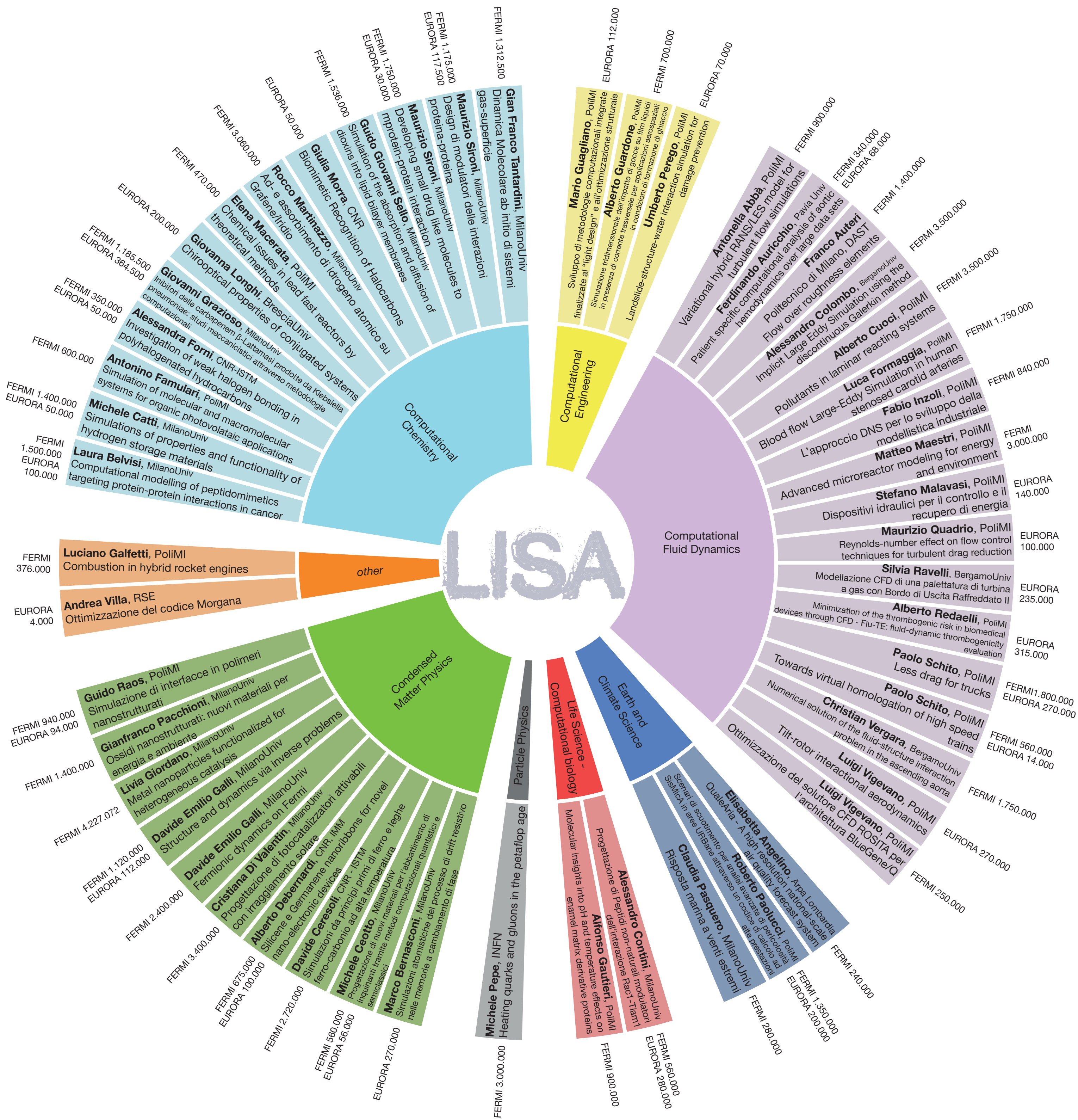
Mapping the conformal window
50.000.000
Gerrit Schierholz, DESY, JSC, Hamburg U, Leipzig U - DE / Adelaide Univ - AU / Riken - JP / Edinburgh U, Liverpool U - UK
Flavor singlets in lattice QCD: sea quark and gluon content of hadrons
16.000.000
Christian Schmidt, BielefeldUniv, RegensburgUniv - DE /Brookhaven National Lab - USA
Fluctuations of conserved charges in the quark gluon plasma
26.000.000
Silvano Simula, INFN, RomeU- IT/BerlinU, BonnU-DE / Valencia U - ES / Paris U - FR / Groningen U - NL
First lattice QCD study of B-physics with four flavors of dynamical quarks
65.000.000 + Jugene
Anastassios Vladikas, INFN,MilanU,RomeU-IT/CERN-CH/ DESY, BerlinU, RegensburgU, MainzU, MuensterU-DE/IFIC, MadridU-ES
Chiral properties of lattice QCD with three dynamical quark flavours
70.000.000
Wolfgang Wenzel, Karlsruhe Institute of Technology - DE/ Mons Univ - BE / CEA - FR / STFC - UK
Multiscale modeling of electronic processes in thin organic films
14.700.000
Giovanni Lapenta, KU Leuven - BE
Space weather effects on the earth environment
10.000.000
Sergio Pirozzoli, Rome Univ - IT
Euler and Navier-Stokes singularities
50.000.000

PRACE
Italian PI
Astrophysics and Universe Sciences
8.400.000 MareNostrum
Marco Baldi
Bologna Univ, INAF Trieste Univ - IT / Munich Univ - DE
Cosmological simulations beyond lambda-CDM
7.700.000 MareNostrum
Salvatore Orlando
INAF, Padua Univ, Palermo Univ – IT
Filling the gap between supernova explosions and their remnants: the Cassiopeia A laboratory
1.800.000 Curie
Franco Vazza
Radio Astronomy Institute - IT / CSCS Lugano - CH / Jacobs Univ Bremen - DE
FERMI - FERMI shedding a new light on Fermi processes in filaments of the Cosmic Web
Biochemistry, Bioinformatics and Life sciences
5.000.000 Curie
Marco De Vivo
IIT – IT
Enhanced sampling simulations to investigate the binding of potent anticancer drugs to the human type II topoisomerase
7.000.000 Curie
Mattia Falconi
Rome Univ -IT / Sao Paulo Univ -BR / Aarhus Univ -DK
Molecular dynamics simulation and experimental characterization of a DNA nanocage family
6.508.160 Curie
Leonardo Guidoni
L'Aquila Univ, Rome Univ - IT
Water oxidation by photosynthesis: dynamics and reactivity of the manganese cluster in the Photosystem II complex explored by quantum mechanics / molecular mechanics simulations
Chemical Sciences and Materials
6.000.000 Curie
Enrico Bodo
Rome Univ - IT
Ab initio molecular dynamics of lanthanides in protic ionic liquids
40.000.000 SuperMUC
Bartolomeo Civalleri
Torino Univ - IT / Montpellier Univ - FR
Ab initio modelling of the adsorption in giant Metal-Organic Frameworks: from small molecules to drugs
8.750.000 SuperMUC
Stefano Corni
CNR, SISSA - IT
All-atom simulation of the Amyloid-beta peptide interacting with gold nanoparticles (AmyGo)
44.744.480 Jugene + Curie
Leonardo Guidoni
L'Aquila Univ, Rome Univ, SISSA - IT
Protein effects on the structural and optical properties of biological chromophores: quantum Monte Carlo / molecular mechanics calculations on Rhodopsin and Light Harvesting Complexes
6.000.000 Curie
Leonardo Guidoni
Rome Univ, L'Aquila Univ, SISSA - IT
Reaction pathways by Quantum Monte Carlo: from benchmarks to biochemistry
38.990.000 Juqeen
Leonardo Guidoni
L'Aquila Univ, Rome Univ, SISSA - IT
Energy storage in the first step of vision explored by quantum Monte Carlo / molecular mechanics calculations
6.500.000 Jugene
Giovanni La Penna
CNR - IT / CNRS - FR
Identification of redox competent species in biological processes
12.000.000 Hermit
Simone Piccinin
CNR, SISSA - IT
Engineering transition-metal multi-core centers in molecular catalysts for solar fuel production
4.816.000 Curie
Simone Piccinin
CNR, SISSA - IT
Multicenter cobalt-oxo cores for catalytic water oxidation
17.000.000 Curie
Sandro Sorella
SISSA - IT / Université Pierre et Marie Curie - FR
Correlation driven phase transitions in Cerium and Cerium-bearing metallic glasses: an ab-initio perspective by quantum Monte Carlo
20.000.000 SuperMUC
Piero Ugliengo
Turin Univ, Modena and Reggio Emilia Univ - IT
Mesoporous silica for drug delivery: a quantum mechanical simulation
Earth System Sciences
53.400.000 SuperMUC
Andrea Morelli
INGV - IT / Toronto Univ - CA
Physics-based evaluation of seismic shaking in Norther Italy
2.977.350 Curie
Daniela Tordella
PoliTo - IT
Fluid turbulence: self and passive scalar diffusion. Application to stably stratified flows
Engineering and Energy
10.500.000 Curie
Paolo Schito
PoliMi - IT / Stanford Univ - USA
Innovative computational methods for wind farms
9.150.160 Hermit
Mauro Sbragaglia
Rome Univ - IT / Eindhoven Univ - NL
Dynamics of multi-component fluid dynamics in porous structures
50.000.000 Jugene
Sergio Pirozzoli
Rome Univ - IT
Structure of turbulence in supersonic boundary layers at high Reynolds number
3.000.000 SuperMUC
Walter Boscheri, Trento Univ - IT
Lagrangian space-time methods for multi-fluid problems on unstructured meshes
Fundamental Physics
35.000.000 Jugene
Vittorio Lubicz
INFN,RomeU-IT/CyprusU-CY/DESY,BerlinU,BonnU,MuensterU-DE / BarcelonaU,ValenciaU-ES/UJF/CNRS/IN2P3,ParisU-FR/ GroningenUniv-NL/LiverpoolU - UK
QCD Simulations for flavor physics in the standard model and beyond
7.700.000 Curie
Arrigo Calzolari, CNR - IT
Ab initio investigation of multidimensional interface between 0D Ag nanoparticle and 1D ZnO wire for optoelectronic applications
3.400.000 SuperMUC
Francesco Califano
Pisa Univ - IT / CNRS - Aix-Marseille Univ - FR
Multi-scale, multi-physics plasma simulations
4.400.000 MareNostrum
Paolo Barone
CNR, L'Aquila Univ - IT / Trinity College Dublin - IE
TRASFER integrating topological order and Rashba-like effects in ferroelectrics
Medicine and Life Sciences
50.000.000 Jugene
Simone Melchionna
CNR – IT
Blood Dynamics in heart-sized coronary arteries
13.000.000 Curie
Stefano de Gironcoli
SISSA, CNR – IT / ICHEC – IE
Structural determination of complex organic/ biological molecular assembly from ab-initio NMR


LISA
Computational Chemistry
Gian Franco Tantardini, MilanoUniv
Dinamica Molecolare ab initio di sistemi gas-superficie
FERMI 1.312.500
Maurizio Sironi, MilanoUniv
Design di modulatori delle interazioni proteina-proteina
FERMI 1.175.000
EURORA 117.500
Maurizio Sironi, MilanoUniv
Developing small drug like molecules to mprotein-protein interaction
FERMI 1.750.000
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Guido Giovanni Sello, MilanoUniv
Simulation of the absorption and diffusion of dioxins into lipid bilayer membranes
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Giulia Morra, CNR
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Rocco Martinazzo, MilanoUniv
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FERMI 3.060.000
Elena Macerata, PoliMI
Chemical issues in lead fast reactors by theoretical methods
FERMI 470.000
Giovanna Longhi, BresciaUniv
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Giovanni Grazioso, MilanoUniv
Inibitori delle carbapenem β-Lattamasi prodotte da Klebsiella pneumoniae: studi meccanicistici attraverso metodologie computazionali
FERMI 1.185.500
EURORA 364.500
Alessandra Forni, CNR-ISTM
Investigation of weak halogen bonding in polyhalogenated hydrocarbons
FERMI 350.000
EURORA 50.000
Antonino Famulari, PoliMI
Simulation of molecular and macromolecular systems for organic photovolataic applications
FERMI 600.000
Michele Catti, MilanoUniv
Simulations of properties and functionality of hydrogen storage materials
FERMI 1.400.000
EURORA 50.000
Laura Belvisi, MilanoUniv
Computational modelling of peptidomimetics targeting protein-protein interactions in cancer
FERMI 1.500.000
EURORA 100.000
Computational Engineering
Mario Guagliano, PoliMI
Sviluppo di metodologie computazionali integrate finalizzate al "light design" e all'ottimizzazione strutturale
EURORA 112.000
Alberto Guardone, PoliMI
Simulazione tridimensionale dell'impatto di gocce su film liquidi in presenza di corrente trasversale per applicazioni aerospaziali in condizioni di formazione di ghiaccio
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Umberto Perego, PoliMI
Landslide-structure-water interaction simulation for damage prevention
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Computational Fluid Dynamics
Antonella Abbà, PoliMI
Variational hybrid RANS/LES model for turbulent flow simulations
FERMI 900.000
Ferdinando Auricchio, Pavia Univ
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EURORA 68.000
Franco Auteri, Politecnico di Milano, DAST
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EURORA 100.000
Silvia Ravelli, BergamoUniv
Modellazione CFD di una palettatura di turbina a gas con Bordo di Uscita Raffreddato II
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EURORA 315.000
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Ottimizzazione del solutore CFD ROSITA per l'architettura BlueGene/Q
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QualeAria - A high resolution national-scale air quality forecast system
FERMI 240.000
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Progettazione di Peptidi non-naturali modulatori dell'interazione Rac1-Tiam1
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Michele Pepe, INFN
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Ossidi nanostrutturati: nuovi materiali per energia e ambiente
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Fermionic dynamics on Fermi
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Cristiana Di Valentin, MilanoUniv
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Alberto Debernardi, CNR, IMM
Silicene e Germanene nanoribbons for novel nano-electronic devices
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Andrea Villa, RSE
Ottimizzazione del codice Morgana
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PRACE

Cineca Supports Studies of Turbulence in the Interplanetary Medium

Living on Earth, and thanks to the support of many space missions, we have the unique opportunity to analyze directly the features of the dynamical behavior of a natural plasma: the interplanetary gas. The interplanetary medium, the so-called solar wind, is a bubble of hot and collisionless fully-ionized gas that is generated by the Sun and fills the Heliosphere.

Our PRACE project has been planned to provide a robust theoretical support, through massive numerical simulations, to the interpretation of observational satellite data in the solar wind on turbulence and magnetic reconnection, two subjects of top priority in space physics. To develop this research activity, we had the unique opportunity to exploit the computational power of the HPC resources provided within the PRACE initiative. Within our project, the numerical hybrid Vlasov-Maxwell (HVM) code [F. Valentini et al., J. of Comput. Phys. 225, 753 (2007)], that integrates the kinetic equation for collision-free protons, has been run on the FERMI machine at Cineca, using a budget of 25 millions CPU hours.

The role of solar-wind turbulence is viewed of primary relevance for channeling the energy from large to short wavelengths, where it can be finally transferred to the plasma particles in form of heat. Our analysis has been focused on pointing out the role of the short-scale kinetic effects, which mainly manifest in the distortion of the velocity distribution (VD) of ions, and the generation of magnetic reconnection events.

In Figure 1 (left) we show the shaded iso-contours in the (x,y) plane, for a fixed z, of the current density together with the perpendicular magnetic field. On the right we show a 3D plot of the proton VD, calculated at a fixed point in the (x,y,z) space corresponding to one of the magnetic reconnection regions. The three-dimensional VD in box (a) displays a potato-like structure and many evident non-Maxwellian signatures. In box (b) we report a cut of the three-dimensional proton VD.

The quantification of the kinetic effects on the proton distribution function has been realized through the analysis of the generation of the temperature anisotropy ($A=T_{\perp}/T_{\parallel}$), with respect to the local magnetic field. In Figure 2, we plot A versus $\beta_{\parallel}$ (ratio of kinetic and magnetic pressure), for a set of solar wind data from the Wind spacecraft (left), and for our numerical runs (right). This plot clearly shows that our model can capture the essential physics of the dynamics of the solar wind protons.

A scientific video, available at www.hpc.cineca.it, containing the description of the main results of the project, has been realized within a PRACE 3IP project and presented at the American Geophysical Union conference (December 2013).

Moreover, a preliminary part of the scientific results obtained has been collected in a number of scientific papers, published in International Journals in 2013.

We wish gratefully thank the PRACE initiative, for providing the opportunity of running massive simulations of solar wind turbulence, and the supercomputing center Cineca for valuable and continuous support to the research activity within this project.

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Francesco Califano
Physics Department, Pisa University

Denise Perrone
Physics Department, Calabria University

Pierluigi Veltri
Physics Department, Calabria University

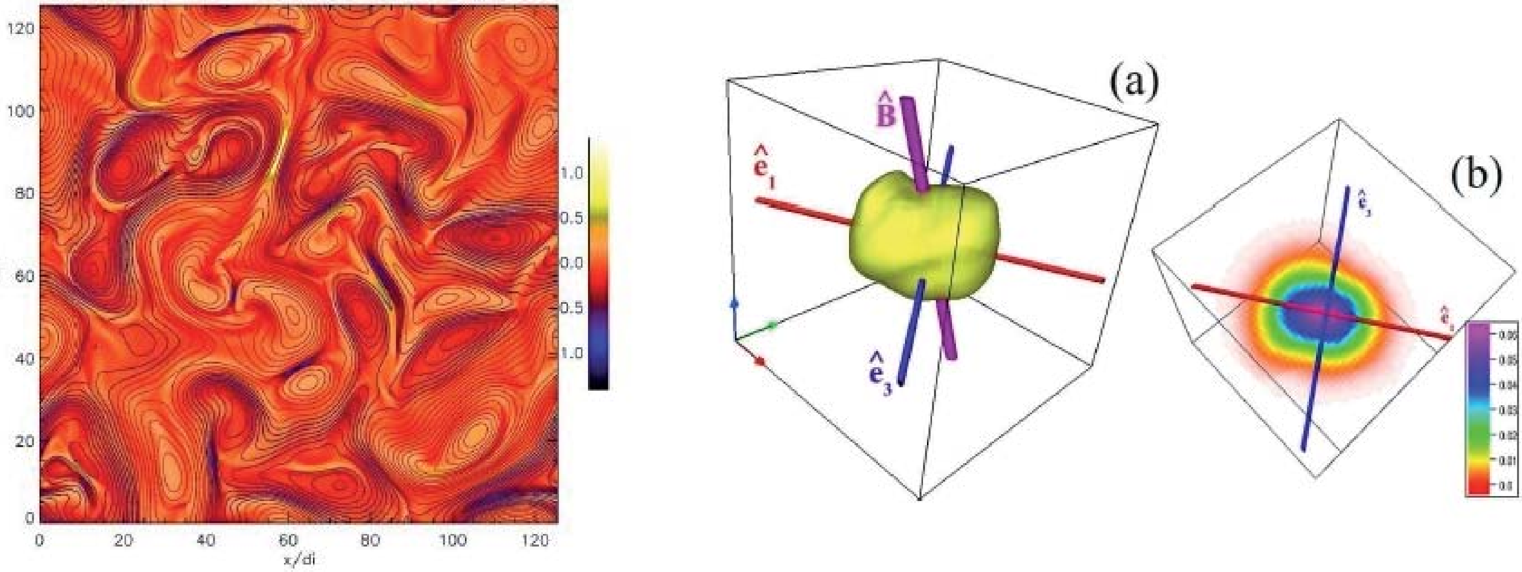
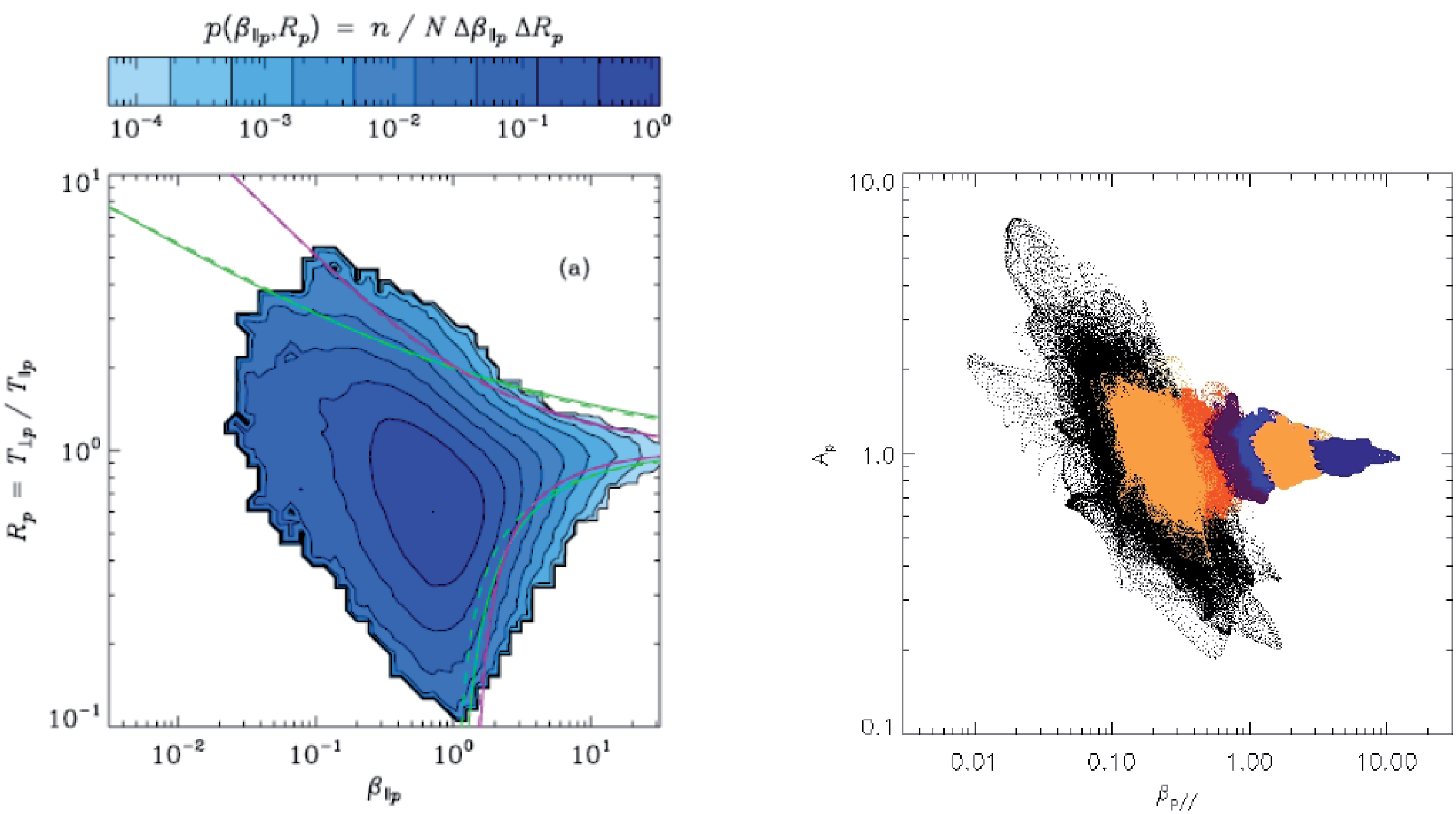


Figure 1:
(left) shaded iso-contours in the (x,y) plane, for a fixed z, of the current density and of the field lines of the perpendicular magnetic field.
(right) 3D plot of the proton VD, at a fixed point in the (x,y,z) space.

Figure 2: Plot of A versus β॥ .
(left) Solar wind data, from the Wind spacecraft [Maruca et al., The Astrophysical Journal 748, 137 (2012)].
(right) numerical results from the HVM simulations.



PRACE

Cineca Resources for Studying the Sun

The Sun is a unique laboratory, since it has extreme ambient conditions and it is the only star that we can resolve in detail.

The question of what heats the solar and stellar coronae to million degrees is very important in Astrophysics and Plasma Physics, because it addresses mechanisms of magnetic energy release and confinement, with implications for research on energy production. Its investigation is very challenging because it involves very different temporal and spatial scales at the same time. The energy is carried from the photosphere by the magnetic field that confines plasma in a multitude of closed magnetic flux tubes, the coronal loops. The PRACE project "The way to heating the solar corona: finely-resolved twisting of magnetic loops" investigates the heating released by the magnetic reconnection of a progressively twisted coronal loop.

Our loop model requires a 3D MHD description with a computation box of more than 10,000,000 grid cells and with millions of time steps. We used the PLUTO 3D-MHD code, and the final simulation required more than 5,000,000 CPU hours on more than 32,000 cores of Fermi BlueGene Q at Cineca. The simulation shows that the twisting triggers a multitude of short-time and localised energy releases that rapidly fill the loop with plasma heated to about 3 million degrees, a typical temperature of solar coronal loops.

The constraints on the heating deposition, e.g. the location and the duration, might be very important for coronal physics.

Our code is highly efficient and optimised for the Cineca BGQ FERMI. This class of resources was not available before and PRACE systems are therefore essential for this and future projects. Cineca's role is highly acknowledged for making FERMI available for a large amount of time that allowed us to perform the simulations.

Due to the complexity of the model, we are still in the process of analysing the results for high impact publications. Preliminary results have been presented in several international meetings (by S. Orlando in PRACE-2IP WP8 Fifth Face to Face MeetingCSCS, Lugano, Switzerland, 6-8/03/2013; F. Reale in Physical Processes in Astrophysical Plasmas Inflow/outflow and stellar winds, Torino, Italy, 12-14/03/2013; F. Reale in 6th Coronal Loop Workshop, 25-28/06/2013, LaRoche, Belgium).

In another investigation, we have studied the impacts of dense fragments erupted after a flare back onto the solar surface, observed in June 2011. The impacts were bright in the EUV band, because - as shown by our hydrodynamic simulations with the FLASH code - they heat the dense and fast impacting fragments to more than 1 million degrees. Our study - published on Science in July 2013 ("Bright Hot Impacts by Erupted Fragments Falling Back on the Sun: A Template for Stellar Accretion") - reports that these impacts are a template for the X-ray-bright impact of accretion flows detected in young stellar systems. The 2D hydrodynamic simulations were run thanks to the ISCRA C project "Testing the formation of accretion shocks in the Sun, after energetic flare eruptions" approved by Cineca in 2012.

Fabio Reale
Palermo University

Salvatore Orlando
INAF - Astronomical Observatory of Palermo

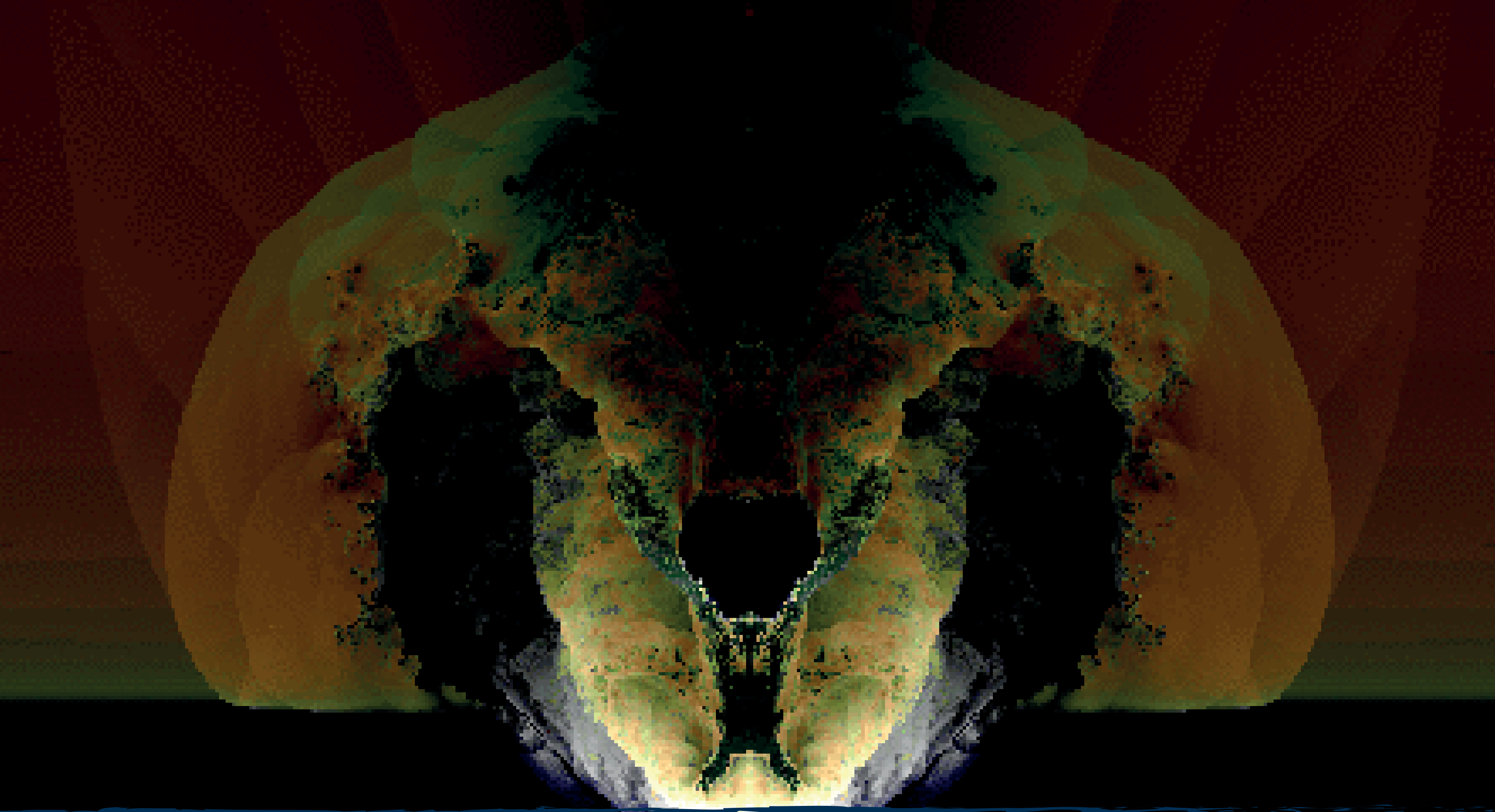
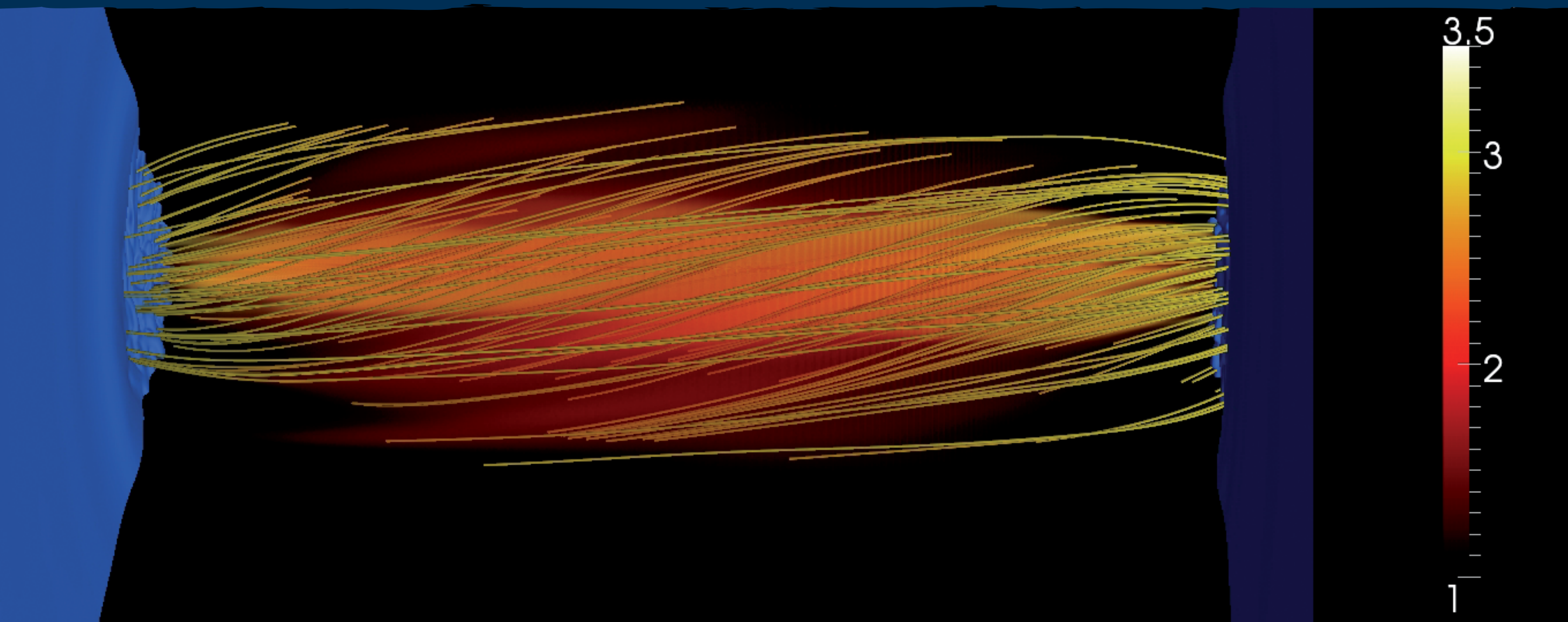


Figure 1: Snapshot during the impact of a train of spherical fragments on the Sun at 400 km/s, as it would be seen by the Solar Dynamics Observatory.
Each color represents the emission (cross-section) in a different band, i.e.171 A (red), 193 A (green), and 335 A (blue). The fragments are dark before the impact, because colder. The impact determines a local heating to about 1 million degrees, that leads everything to be visible in the Extreme UltraViolet band.
The 2D hydrodynamic simulation is performed with the FLASH code.

Figure 2: 3D volume rendering of the temperature in a twisted coronal magnetic flux tube after many heating releases due to the reconnection of the twisted magnetic field lines. The central part of the domain is heated to more than 3 million degrees. The magnetic field lines are also shown and are clearly strongly twisted. The blue region is the chromosphere. The 3D MHD simulation is performed with the PLUTO code.



PRACE

Novel Materials for Artificial Photosynthesis

The discovery and optimization of novel materials for artificial photosynthesis can impact on two of the most urgent problems faced by mankind: energy and environment. The ultimate goal of artificial photosynthesis is the conversion and storage of solar energy into high-energy chemical fuels.

In artificial leaf technologies, the overall reaction entails a sequence of light-promoted electron and proton transfers coupled with cleavage and formation of molecular bonds, ultimately splitting H_2O molecules into higher energy products as O_2 and H_2 ($2H_2O \rightarrow O_2 + 4H^+ + 4e^-$). A technological bottleneck is the design and optimization of innovative catalysts for the half reaction of water oxidation. Catalyzing this reaction with high quantum efficiency, low over potential, high turnover frequencies, and without deactivation, is a formidable challenge because of its high thermodynamic cost and mechanistic complexity.

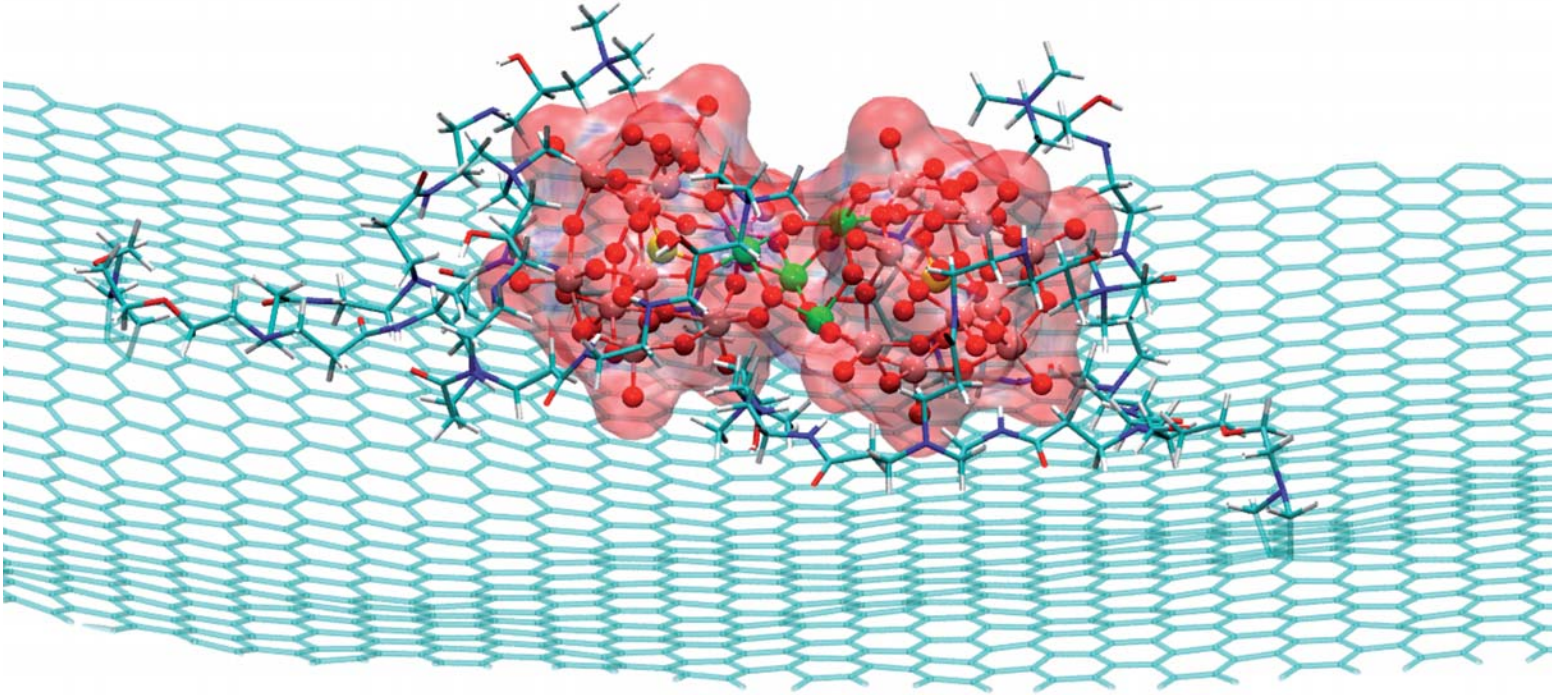
Finding stable catalysts capable of promoting water-oxidation efficiently and with low thermodynamic losses is extremely challenging and is presently undertaken with combined experimental and theoretical approaches, in which numerical materials modeling plays a key role.

The Cineca ISCRA-A project “Functionalized carbon nanotubes for artificial photosynthesis” addressed novel multicomponent anodic materials consisting of Ru-based inorganic molecular complexes anchored on functionalized carbon nanotubes. Little is known on how these molecular complexes bind to the electrodes and how the interfaces affect the function of the device. The complexity of the systems together with the presence of the solvent required combining different levels of theory and computational techniques, all of them involving several hundreds of atoms (~400 atoms for the catalyst system and at least 3000 water molecules). A meaningful numerical modeling of this system could only be achieved by the computational resources provided by Cineca. Our study provided the first detailed atomistic model of the electrode/catalyst interface (Fig. 1) and showed that the catalytic efficiency of this heterogeneous catalysts is not worsened by its binding to the electrode.

The PRACE project “Shedding light on the catalytic core of artificial leaf technologies” focused on a class of materials - cobalt-phosphate (Co-Pi), cobalt-borate, nickel-borate, and others - that have been recently discovered and successfully applied to artificial leaf technologies. Their activity relies on ordered and oxidation-resistant active centers embedded in amorphous grains. The structure of these active cores is debated and experimentally elusive because of the complex amorphous structure and composition of the grains. Our computational study provided the first realistic and statistically meaningful structural model of the Co-Pi catalyst, and opened the way for understanding the functionality of these catalysts. We have determined the stability and structure in solution of realistic nanoparticles and are currently investigating the water oxidation and O-O bond formation.

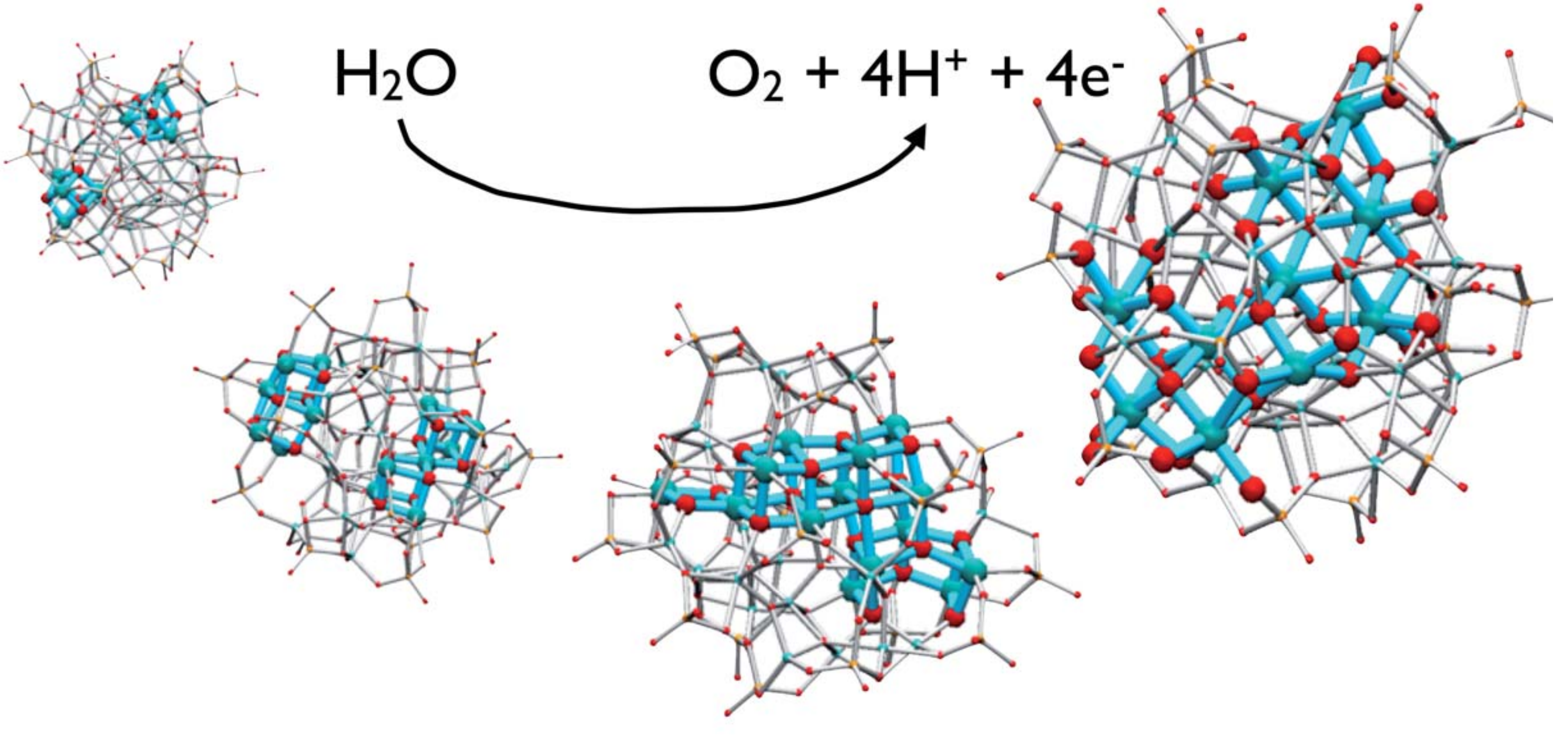
In summary, the computing resources and technical assistance provided by Cineca have allowed to identify important correlations between the mechanism of reaction, thermodynamic efficiency, and local structure of the active sites. These results can guide the rational design of superior catalysts.

Stefano Fabris
CNR-IOM DEMOCRITOS



Figue 1: Snapshot of molecular dynamics simulations showing the binding configuration of Ru-polyiximetalate catalyst to functionalized graphene electrodes.

Figure 2: Structural models of amorphous cobalt-phosphate nanoparticles identified with metadynamics calculations. The simulations show the formation of ordered cubane crystallites in the amorphous matrix.



ISCRA

Cineca for Seismological Studies

Seismic shaking is highly influenced by wave propagation effects: sedimentary basins are known to amplify specific frequencies, while 3D geological structures can focus or de-focus seismic energy. This results in significant variation of ground motion even on small scales. Therefore, reliable seismic hazard estimates for a specific location also depend on knowledge of the response of geological structure to radiated elastic energy. On the other hand, the observation, at the surface of the Earth, of the wave field perturbed by propagation in the heterogeneous medium, permits the reconstruction of the deep internal structure of the planet through seismic tomography.
Realistic calculation of seismic ground motion is possible by using numerical solvers of the elastic wave equation. Spectral element solvers are particularly attractive due to their efficiency (e.g., SPECFEM3D, Komatitsch & Tromp, 2002; Peter et al., 2011). They enable full-waveform inversion, a technique still in its infancy, that holds great promise for the future: extracting more information from the seismograms means retrieving more detailed models of the deep structure of the Earth, that in turn will allow a better understanding of its dynamic processes.
In our research projects, we directed our attention to the Po Plain region, where high property and industrial exposure increases the damaging potential of seismic shocks - as shown by the impact of the 2012, May 20th and 29th, earthquakes. Realistic simulations including the frequency range of relevance for engineering purposes require a detailed knowledge of the geological structure and its accurate representation. These simulations require massive computational resources, that we can only access thorugh ISCRA grants. Our goal is to produce estimates of expected ground shaking in Northern Italy through detailed deterministic simulations of ground motion due to expected earthquakes.
We also study the structure of the only region of deep seismicity in Europe, the Vrancea (Romania) region, to understand its connection with fossil subduction and presence of a remnant of lithospheric slab at depth. Our project consists of implementing the full waveform inversion method in a tomographic reconstruction, where the 3D structural model is iteratively updated through estimates of the gradient of the misfit function obtained by the adjoint method.
These studies are still in their development, but have already produced some significant results that have been presented at international conferences, and that are being published on scientific literature. One important outcome of the studies that have been supported by ISCRA at Cineca, is their preparatory significance for obtaining a currently ongoing PRACE grant to access Tier 0 resources, needed to realize large-scale simulations to update and validate the geological model of the Po Plain.
We wish to thank the ISCRA program for permitting access to the Cineca high-performance computing center, enabling these computationally-intensive seismological studies.

Andrea Morelli
INGV, Bologna

Irene Molinari
INGV, Roma1

Julie Baron
INGV, Bologna

Peter Danecek
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Piero Basini
Physics Department, Toronto University

Paride Legovini
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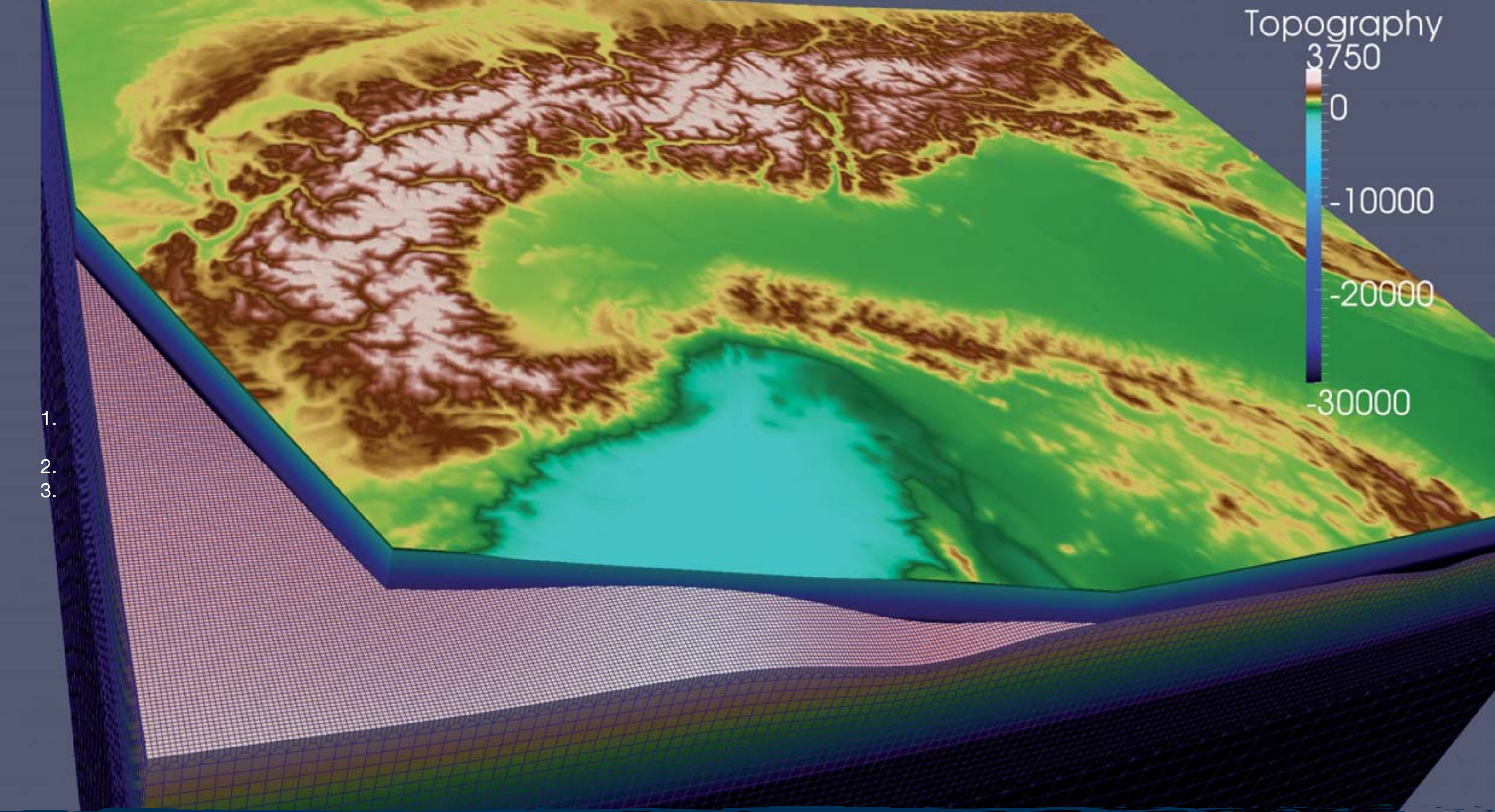


Figure 1: Mesh of the crust and the mantle, colored as a funcion of the topography. The mesh has element size of 2 km in the crust, and has about 3 million elements.

Figure 2: Snapshots of the simulation of the 2013, June 21, M=5.2 Lunigiana earthquake. The effect of the basin structure is apparent when the wave front passes the ESE-WNW-trending boundary with the mountain front.

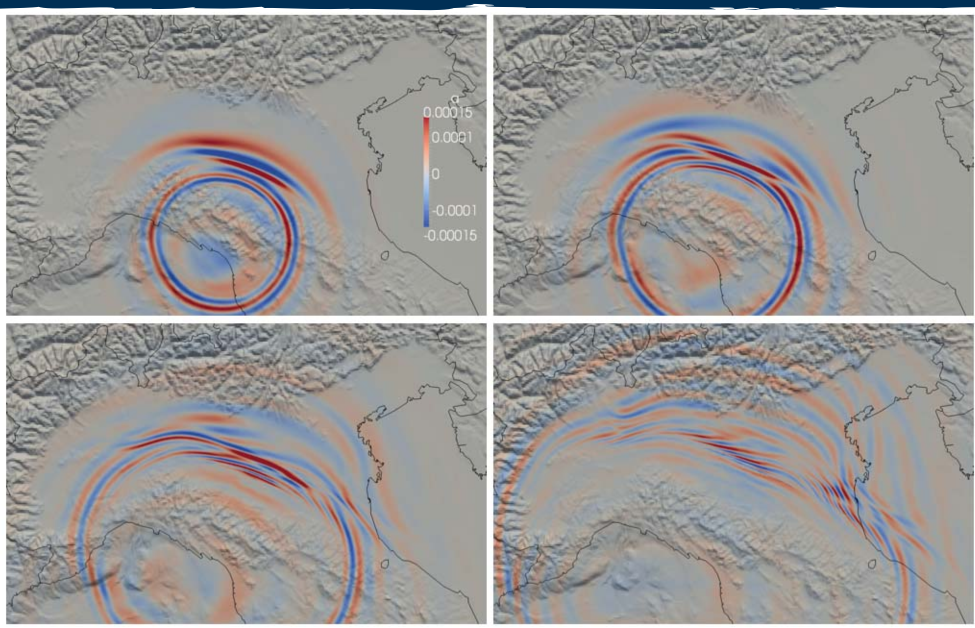
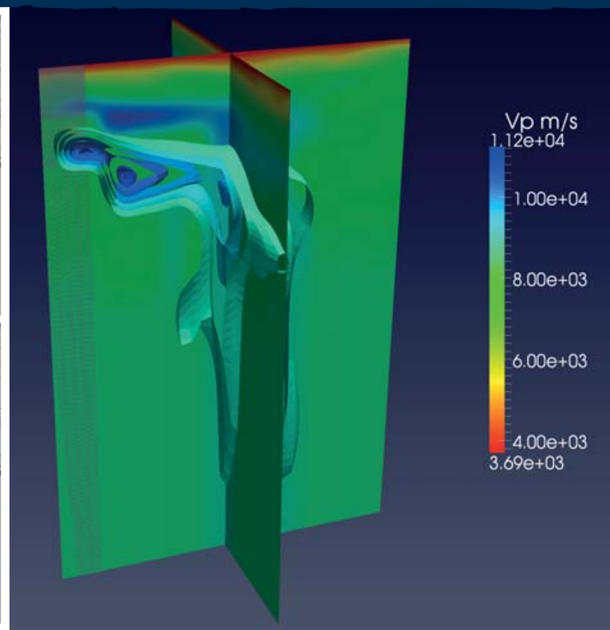


Figure 3: Three-dimensional rendering of iso-surfaces of seismic wave velocity in the Earth's mantle below the Vrancea (Romania) lithospheric subduction zone.



ISCRA

HPC for Medical Science: an Atomistic Model Describes Diabetes

The human islet amyloid polypeptide (hIAPP) is the primary component in the toxic islet amyloid deposits in type-2 diabetes. hIAPP self-assembles to aggregates that permeabilize membranes and constitutes amyloid plaques. Uncovering the mechanisms of amyloid self-assembly is the key to understanding amyloid toxicity and treatment. Although structurally similar, hIAPP's rat counterpart, the rat islet amyloid polypeptide (rIAPP), is non-toxic. It has been a puzzle why these peptides behave so differently. We combined multiscale modelling and theory to explain the drastically different dynamics of hIAPP and rIAPP:
We have performed multiscale computer simulations, in time scales of tens of microseconds, to study the interactions of hIAPP and its rat counterpart (rIAPP) with phospholipid membranes. The simulations, running on Italian (Cineca) and Canadian (SharcNet) HPC computational resources, were performed in a membrane environment - peptide aggregation and changes in secondary structure occur differently in aqueous solution and in membranes, the latter being the physiologically most important case. We also developed a thermodynamic model to study aggregate formation and morphological changes. Using theory and simulations, we explain the physical mechanisms behind the different modes of aggregate formation and peptide-membrane interactions of hIAPP and rIAPP. The predicted diameter of the water pores formed by peptides and the number of peptides agrees well with experiments.
In the article on Nature Scientific Reports (DOI: 10.1038/srep02781) we presented this atomistic model for explain molecular events from onset to propagation of type-2 diabetes or diabete Mellitus. This important result help to plain new drugs for prevent diabetes.

Martina Pannuzzo
Erlangen-Nuremberg University, Germany

Antonio Raudino
Catania University, Italy

Danilo Milardi
CNR, Catania, Italy

Carmelo La Rosa
Catania University, Italy

Mikko Karttunen
Waterloo University, Canada

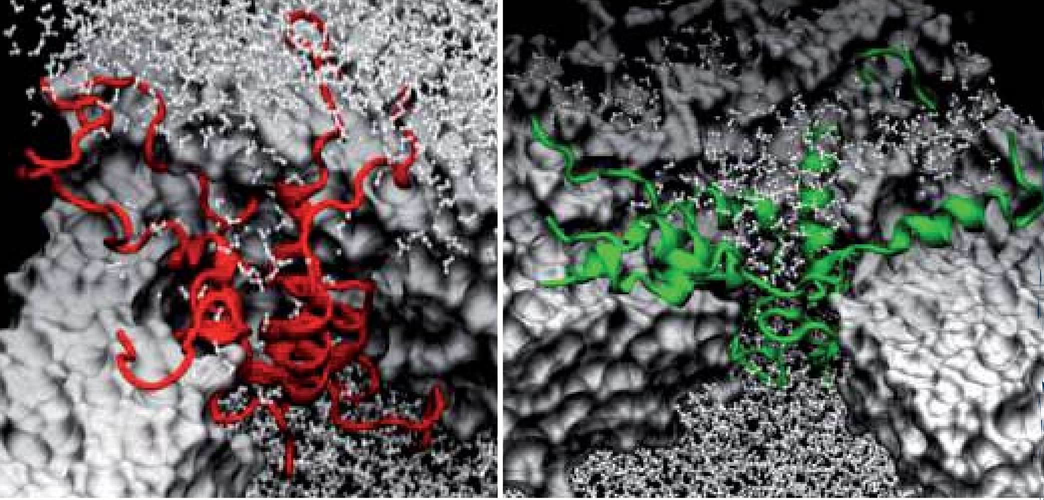


Figure 1:
hIAPP pentamers resemble barrel-shaped channels whereas the corresponding rIAPPassemblies look like loose funnels. Snapshots from AA-MD simulations of IAPP (red) and rIAPP (green) pentamers after 300 ns. Color code: white-surf-lipids, white-CPK-water.

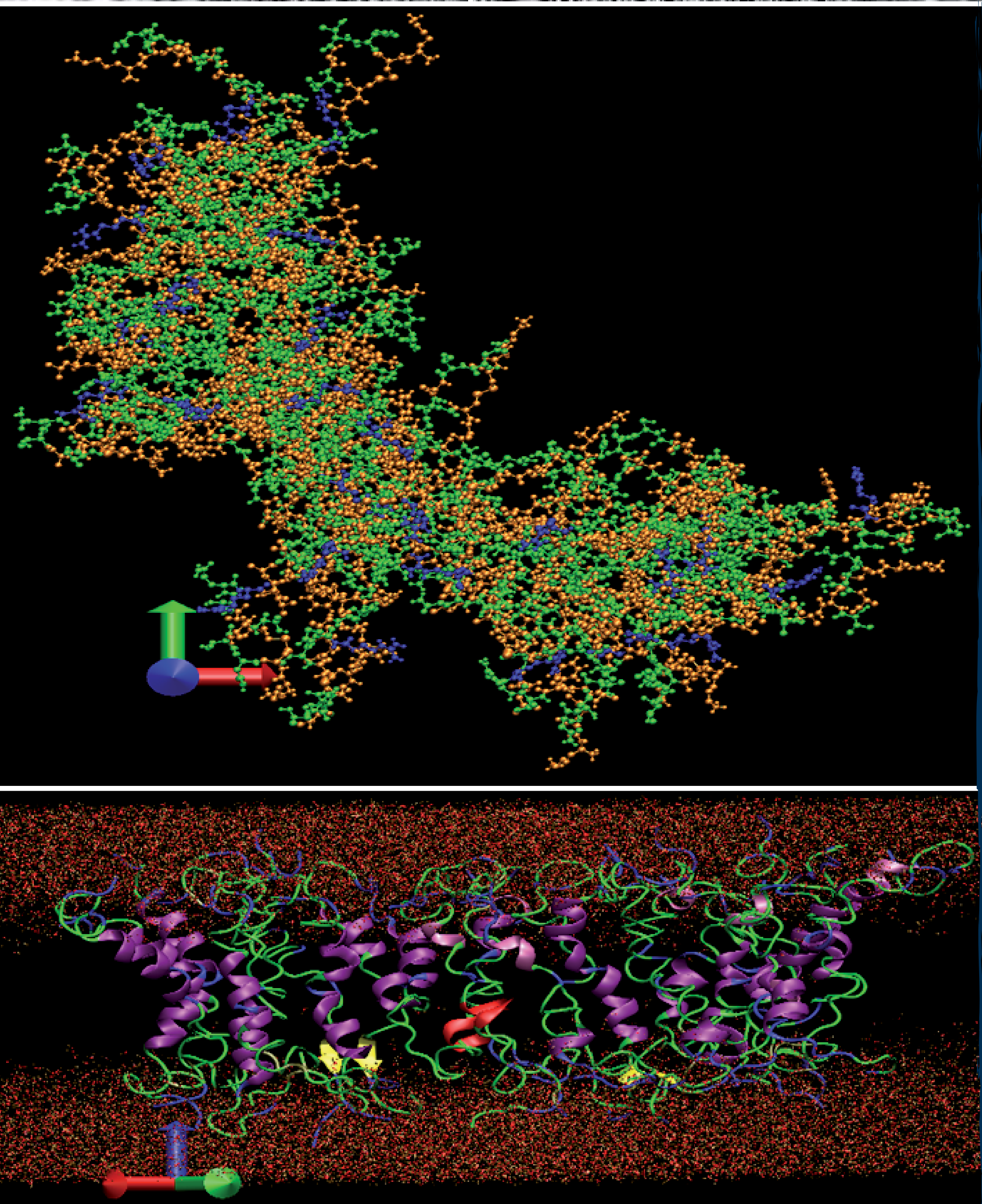


Figure 2:
Upper panel. Top view of the structure of the semi-toroidal aggregate formed by 26 hIAPP molecules after 20 ns of AA simulation at 300 K. Lower panel. Side view of the aggregate. α-helices are represented in purple, random-coils in green and β-sheets in yellow.

LISA

Initiative for a Virtual Wind Tunnel

The research projects regarding the use of HPC resources in the Department of Mechanical Engineering of Politecnico di Milano involve the synergy between the experimental wind tunnel and the computational fluid dynamics approach. The main LISA project of the Department of Mechanical Engineering was dedicated to the reproduction of the atmospheric boundary layer (namely the natural wind) that is realized in the wind tunnel (see Figure 1) for the analysis of several aerodynamic issues: high speed winds may cause damage to buildings, bridges, vehicles and wind turbines. Specifically, the interaction between wind and wind turbines is not related only to safety issues, but concerns also wind energy production and the management of the wind turbine itself. The wind tunnel was used to validate the numerical models developed during the LISA project comparing the experimental data with the numerical results. The advantage of a validated numerical model is not only the possibility to have an easy access to all quantities that are otherwise not easily measurable during experiments, but also to design numerical experiments that are difficult to realize with real models. A very interesting result that was achieved is the calculation of the wake of a wind turbine (see Figure 2): this information is not so important when dealing with a single wind turbine but it becomes of fundamental interest when considering an entire wind farm. Wind turbines in a wind farm interact with the upstream wind turbine wakes, and this will affect both the power production and the mechanical and structural stresses on their structure.

More than 1 million CPU hours were dedicated to the study of the interaction of the natural wind with wind turbines, more than 10 publications, several master theses and one PhD thesis were produced thanks to the LISA calls.

The LISA initiative and Cineca staff support gave to the Department of Mechanical Engineering HPC research activity the possibility to grow to a European scale, since thanks the LISA initiative the development of the wind turbine research project submitted on the PRACE platform has been awarded by grant n.2012061147 with more than 10 millions CPU hours.

Paolo Schito
Politecnico di Milano

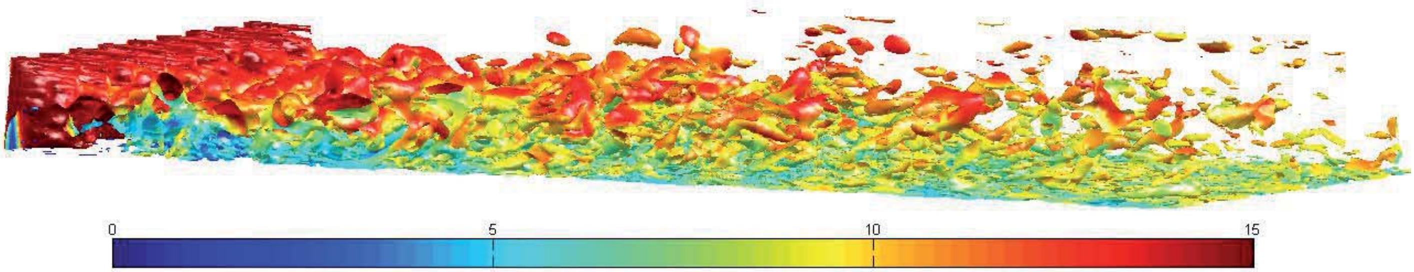
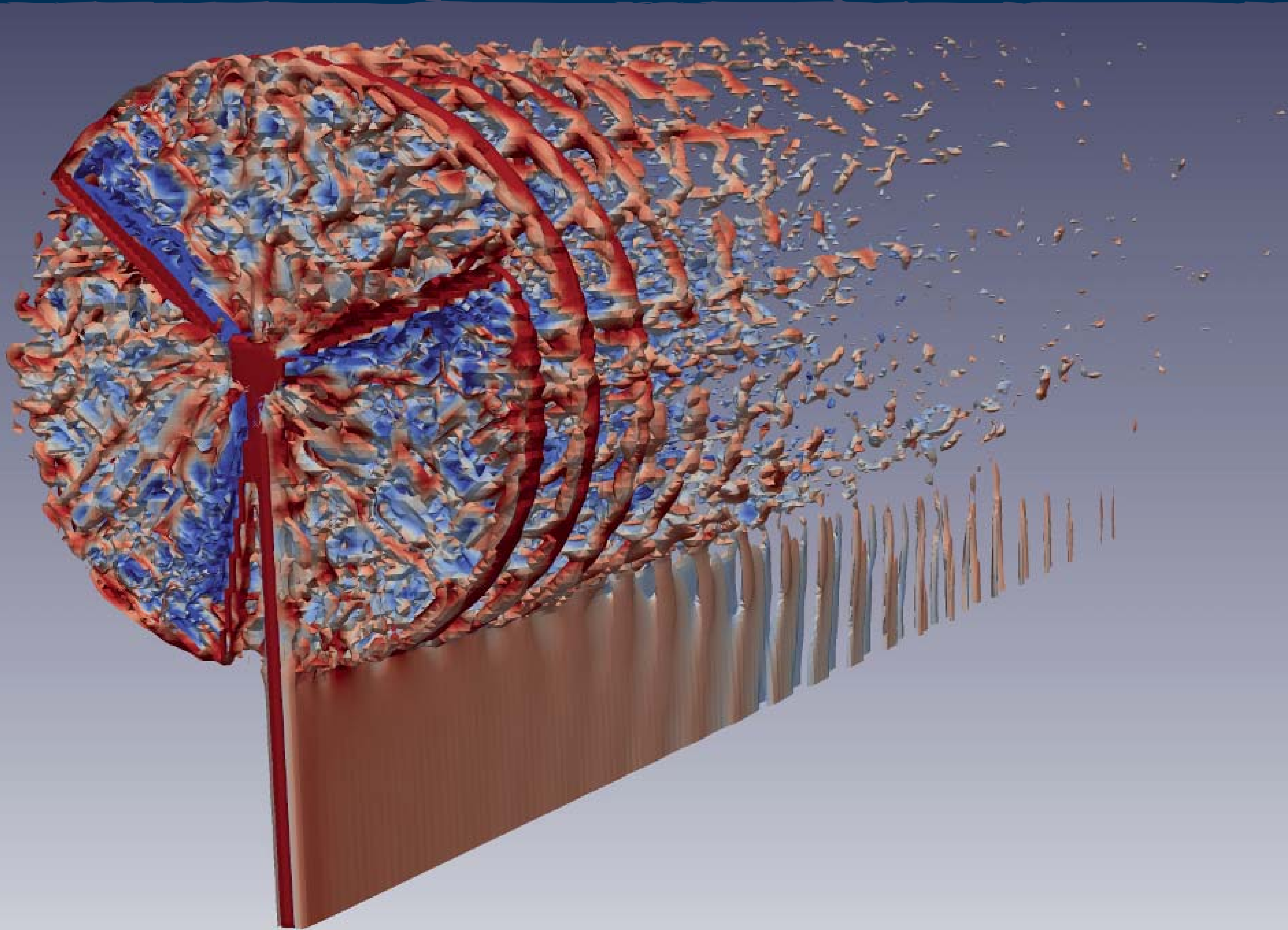


Figure 1: Numerical calculation of the turbulent flow realized in the wind tunnel of Politecnico di Milano: it is possible to see the turbulence structures colored with the local speed of the wind.

Figure 2: Numerical calculation of the wake of a wind turbine. It is possible to distinguish the turbulence structures originated by the interaction of the blades with the incoming flow and their evolution and dissipation downstream.

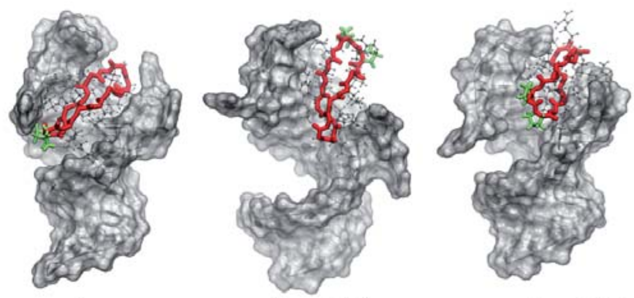


ISCRA

RNA-protein binding by means of massively-parallel biased simulations

Giovanni Bussi
SISSA - ISAS

RNA/protein interactions play crucial roles in controlling gene expression. They are becoming important targets for pharmaceutical applications. Due to RNA flexibility and to the strength of electrostatic interactions, standard docking methods are insufficient.
We have developed a computational method which allows studying the binding of RNA molecules and charged peptides with accurate atomistic, explicit-solvent molecular dynamics. In our method, a suitable estimate of the electrostatic interaction is used as an order parameter (collective variable) which is then accelerated using bi-directional pulling simulations [1].
We have applied this method to characterize the binding of TAR RNA from HIV-1 and a small cyclic peptide. In particular, we performed pulling simulations where we drive our collective variable from zero (unbound state) to a negative value (bound state) and back, thus inducing binding and unbinding of the complex. Many steering simulations are performed in parallel, each of them running on several processors.
Our simulation protocol allows blindly predicting the binding pocket and pose as well as the binding affinity. One of the predicted poses is in remarkable agreement with the experimentally obtained structure [2]. The method is general and could be applied to study other electrostatics-driven binding events.



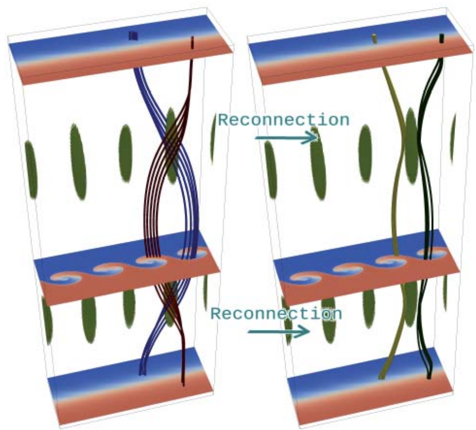
Experimental structure of the RNA/peptide complex (left). Two of the predicted structures (center and right). Structure (2) is in remarkable agreement with experiment, and has been obtained blindly, i.e. without exploiting any information about the binding site and pose.

[1] Do, Carloni, Varani, and Bussi, J. Chem. Theory Comput. 2013, 9, 1720
[2] Davidson, Leeper, Athanassiou, Patora-Komisarska, Karn, Robinson, and Varani, Proc. Natl. Acad. Sci. U. S. A. 2009, 106, 11931

Multi-scale Plasma Simulations - MPS

Francesco Califano
Physics Department, Pisa University

We investigate with 3D two-fluid simulations the Solar Wind interaction with the Magnetosphere at low latitude. When the solar wind magnetic field is northwards, the Kelvin-Helmoltz instability generates a vortex chain eventually disrupted by secondary instabilities.
Our main result is the completely different dynamics of the system with respect to the standard 2D approach: K-H vortices developing at the equator become an energy source for the dynamics far from the equatorial region by creating extended current sheets at mid-latitudes where magnetic reconnection occurs spontaneously. Magnetic flux tubes connected to the Earth at both poles but embedded in the solar wind, are created which could explain the entry of solar wind plasma into the magnetosphere.
The code integrates the two-fluid plasma equations in a 3D slab geometry using the IV order Runge-Kutta scheme in time and a VI order Compact Finite Difference Scheme for derivatives along the open x-direction and VI order Explicit Finite Difference Scheme along the periodic y and z-directions. Numerical stability is achieved by means of filters. The code parallelized with MPI runs on the BG/Q Fermi Machine at Cineca. Typical grid size ~ 10003. A production run takes about 106 hours.

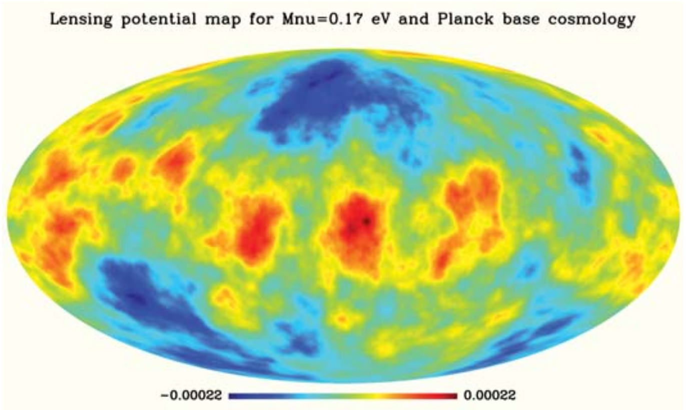


Magnetic Reconnection at mid-latitude.

Dark-Energy and Massive-Neutrino Universe Simulations

Carmelita Carbone
INAF - Astronomical Observatory of Brera

Neutrinos represent the only dark matter particle that has been actually detected and directly studied. It is now established from solar, atmospheric, reactor and accelerator neutrino experiments that neutrinos have non-zero mass, with a lower limit on the total neutrino mass Mnu=0.058 eV. This is a clear indication that the standard model of particle physics is incomplete. Since a thermal neutrino relic component in the Universe impacts both the expansion history and the growth of structure, cosmological probes are very sensitive even to very small neutrino masses. In order to explore the effects of massive neutrinos on cosmic structure formation on a very large range of scales, within the ISCRA awarded class-A project entitled "Dark Energy and Massive Neutrino Universe" (DEMNUni), we have produced the largest cosmological N-body simulations with a neutrino particle component ever present in the literature. They are characterised by box-side L=2 Gpc/h, particle number Npart=2x2048^3 and a base Planck cosmology with Mnu=0, 0.17, 0.3, 0.53 eV. With this large set of simulations we are producing very large mock galaxy catalogs, cosmic-shear maps, and CMB-lensing maps, that take into account massive neutrino effects and mimic the sky observed by future probes as EUCLID and PRISM. The importance of this project lies on the necessity of producing future probes end-to-end simulations which do take into account neutrino effects.

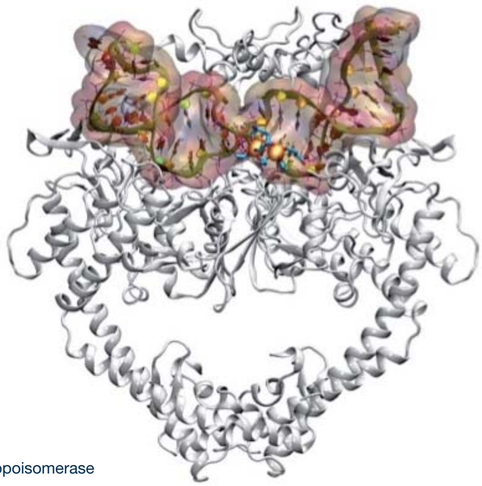


Example of all-sky CMB lensing maps, produced by ray-tracing across the matter distribution of one of the DEMNUni simulations.

Enhanced sampling simulations to investigate the binding of potent anticancer drugs to the human Type II topoisomerase

Marco De Vivo
Italian Institute of Technology

This project aims at investigating function and inhibition of type II topoisomerase (topoII). TopoII controls the topology of DNA in all cells and are important targets of clinical antibiotics and anticancer agents.
Based on recent crystal structures of the topoII-DNA-drug complex, we propose to employ state-of-the-art computational methodologies to understand the binding mode and key interactions of potent anticancer drugs, such as etoposide.
These simulations will return a detailed picture of the free energy landscape of drug binding to topoII, highlighting also how certain topoII mutations are able to induce drug-resistance. Clarification of the dynamics of the catalytic site structural determinants of topoII during drug binding could also offer useful insights for the rational structure-based design of new anticancer and antibacterial drugs.

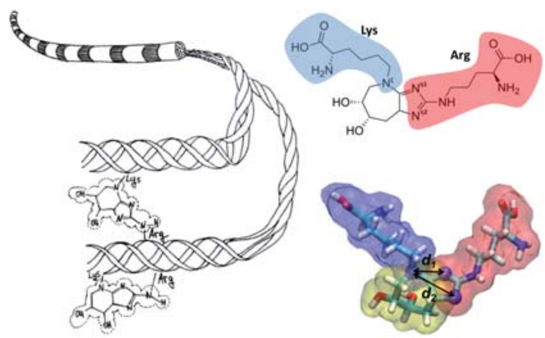


Type II Topoisomerase

Age-and diabetes-related nonenzymatic crosslinks in collagen fibrils: candidate amino acids involved in Advanced Glycation End-products

Alfonso Gautieri
Politecnico di Milano

Ageing and diabetes share a common deleterious phenomenon, the formation of Advanced Glycation Endproducts (AGEs), which accumulate predominantly in collagen due to its low turnover. Though the general picture of glycation has been identified, the detailed knowledge of which collagen amino acids are involved in AGEs is still missing. In this work we use an atomistic model of a collagen fibril to pinpoint, for the first time, the precise location of amino acids involved in the most relevant AGE, glucosepane. The results show that there are 14 specific lysine-arginine pairs that, due to their relative position and configuration, are likely to form glucosepane. We find that several residues involved in AGE crosslinks are within key collagen domains, such as binding sites for integrins, proteoglycans and collagenase, hence providing molecular-level explanations of previous experimental results showing decreased collagen affinity for key molecules. Altogether, these findings reveal the molecular mechanism by which glycation affects the biological properties of collagen tissues, which in turn contribute to age- and diabetes-related pathological states.



Collagen fibril and glucosepane. Left panel shows a schematic of collagen fibril and the formation of glucosepane, which covalently links Lysine and Arginine sidechains. The two amino acids can belong to separate molecules, forming an intermolecular crosslink, or to the same molecule. Panel on top left shows the chemical structure of glucosepane, which crosslinks lysine (blue) to arginine (red). P anel on bottom right shows the molecular model of glucosepane, used to evaluate the distances between the terminal atoms of the two residues ($d_1 \approx 2.6$ Å, $d_2 \approx 3.8$ Å).

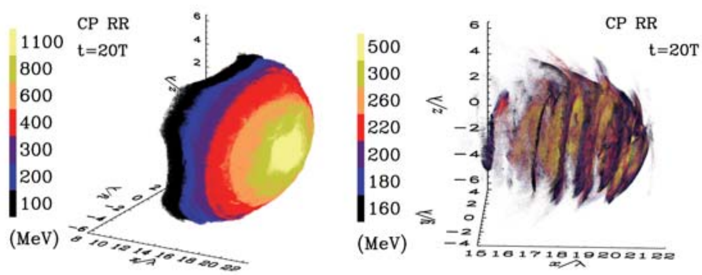
Towards Full-Scale Simulations of Laser-Plasma Experiments

Andrea Macchi
INO - CNR

The TOFUSEX (TOwards FUll-Scale simulations of laser-plasma interaction EXperiments) project has been devoted to the numerical simulation of superintense laser-plasma interactions using kinetic, relativistic, fully electromagnetic particle-in-cell codes.

The main aim was to perform more realistic (three-dimensional, high resolution, long space and time scales) simulations to support the design and interpretation of present and future experiments.

The ISCRA award allowed in particular to perform probably the most accurate 3D simulations so far of the direct light pressure acceleration regime as well as the first ones including radiation friction effects.



Sailing before the light: three-dimensional particle-in-cell simulations of the acceleration of a thin plasma foil by the radiation pressure of a superintense laser pulse. The figure shows the spatial distribution of ions (left) and electrons (right) with colors giving the energy in MeV.

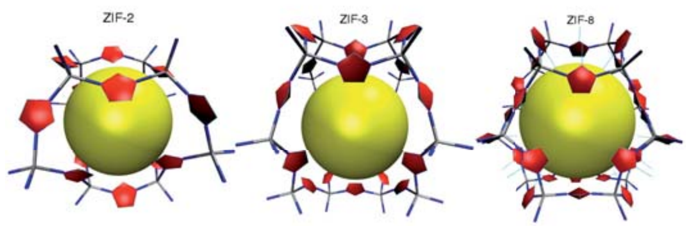
M. Tamburini, T. V. Liseykina, F. Pegoraro, A. Macchi, Radiation Pressure Dominant Acceleration: Polarization and Radiation Reaction Effects and Energy Increase in Three Dimensional Simulations, Physical Review E 85, 016407 (2012)

ISCRA

Theoretical Insights of CO2 Storage and Separation in Zeolite Imidazolate Frameworks with Ab initio Molecular Dynamics Simulations

Marco Masia
Chemistry and Pharmacy Dept., Sassari University

In this work we have studied the electronic properties and the absorption mechanism of Zeolite Imidazolate Frameworks (ZIFs), novel porous materials that are characterized by interesting absorption properties, which makes them good candidates for carbon dioxide sequestering. The electronic properties of these materials have been studied through ab initio calculations, both with quantum chemical methods and with first principles Molecular Dynamics simulations. The information thus obtained has been used for Grand Canonical Monte Carlo simulations to model the behavior of three different ZIFs, with particular emphasis on the absorption isoterms. The ab initio study (performed both on clusters and on periodic systems) allowed us to obtain information about the structure, and about the electronic density. By fitting the ab initio electrostatic potential we found that charge fluctuations in ZIF-2, ZIF-3 and ZIF-8 are very narrow, therefore justifying the use of the point charge approximation for these materials [J. Chem. Theory and Comput. (2011) 7, 1575]. We also found that the regions proximal to the linkers (molecules coordinating zinc ions) are the preferential adsorption sites for carbon dioxide, and that The uptake capacity at low pressures is related to the electrostatic interaction of the adsorbate with the crystal [Chem. Phys. Lett. (2013) 580, 99].

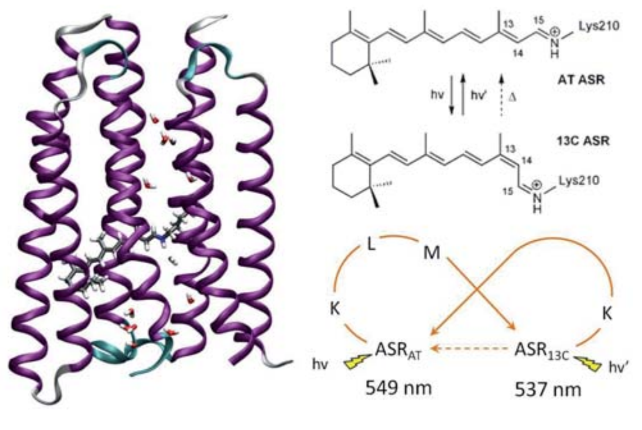


Crystalline geometries of ZIF-2, ZIF-3, and ZIF-8 with large cages shown by yellow spheres. Repeating Square-hexagonal, Square-octagonal, and Square-hexagonal small cage sites are also shown.

Computational Engineering and Prediction of Excited State Properties of Bacterial Photoreceptor Mutants

Massimo Olivucci
Siena University

Anabaena Sensory Rhodopsin (ASR) is a photochromic rhodopsin from the cyanobacterium Anabaena (Nostoc) sp. PCC7120, whose two stable ground state isomers, feature an all-trans (ASR_{AT}) and 13-cis (ASR_{13C}) configuration of its retinal chromophore. Their photochemical interconversion was shown to be ultrafast (<150 fs) for 13C→AT and slower (>500 fs) for the reverse reaction. The wild type and the 2 mutants Trp76Phe and Leu83Gln were computationally studied by means of a hybrid multiconfigurational quantum mechanics / molecular mechanics (QM/MM) approach to evaluate the effect of mutations on spectroscopy and reactivity, for which excited state molecular dynamics was used. Mutations have a large effect on the time required to reach the conical intersection of excited and ground states mediating the reaction: Trp76Phe slows down the reaction, while Leu83Gln accelerates it. These effects can be ascribed to different electrostatic effects of the newly introduced residue onto the chromophore. Since a positive charge transfer occurs on retinal excited state, the removal (Trp76Phe) or addition (Leu83Gln) of a dipole changes the reaction profile, thus leading to the computed outcomes. This study demonstrates that computed mutant models can help to engineer biological systems with desired optical properties.



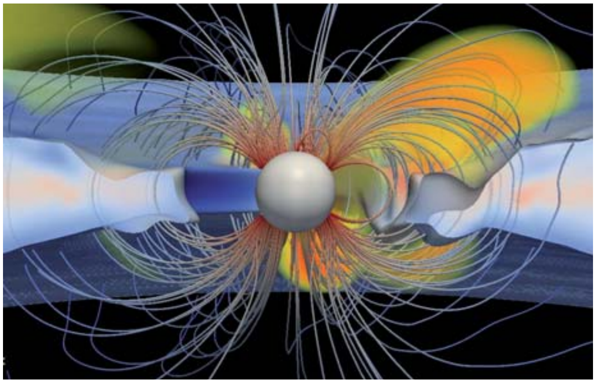
Anabaena Sensory Rhodopsin: structure and photochemical cycle.

Mass accretion onto young stellar objects driven by flaring activity in protostellar disks

Salvatore Orlando
INAF - Astronomical Observatory of Palermo

According to the magnetospheric accretion scenario, young low-mass stars are surrounded by circumstellar disks which they interact with through accretion of mass. The accretion builds up the star to its final mass and is also believed to power the mass outflows, which may in turn have a significant role in removing the excess angular momentum from the star-disk system. On the other hand, strong flaring activity is a common feature of young stellar objects (YSOs). In the Sun, such events give rise to perturbations of the interplanetary medium. Similar but more energetic phenomena occur in YSOs and may influence the circumstellar environment. In the framework of a recent ISCRA A project (HP10A4ZCV5), we challanged the idea that an intense flaring activity close to an accretion disk may perturb the stability of the disk and trigger mass accretion onto the star. We performed 3D MHD simulations describing a rotating magnetized star surrounded by a thick quasi-Keplerian disk; a storm of flares is distributed randomly in proximity of the disk surface.

The simulations have shown that bright flares occurring close to the circumstellar disk can trigger substantial and persistent accretion flows; an intense flaring activity in proximity of the disk determines the formation of an extended corona linking the star with the disk.



Effects of a storm of flares on the disk stability. Cutaway view of the star-disk system showing the mass density of the disk (light blue). The panel overplot the three-dimensional volume rendering of the plasma temperature, showing the flaring loops (in red) linking the inner part of the disk with the star. Selected magnetic field lines are overplotted.

Helical switch design from free energy methods

Adriana Pietropaolo
Catanzaro University

Chiral emitting polymers with switchable screw sense are versatile frameworks for chiral functional materials.[1,2] Starting from ISCRA and thereby within the PRACE framework, we worked on the reconstruction of the free energy landscape of a class of polymers which selectively revert its handedness upon CPL irradiation.

We succeed in reporting the first free energy surface reconstruction on helix polymer reversal[3] along a chiral reaction path based on the combination of path collective variables[4] and chirality indexes.[5-7] The free energy simulations reproduced the experimental electronic circular dichroism spectra. The simulation method developed owing to ISCRA and PRACE resources can be expanded to a wider variety of macromolecular systems that undergo a large-scale structural transition. Future perspectives will be put to selectively obtaining devices with bespoke activation barriers.

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(5) Osipov, Pickup, Dunmur, Mol. Phys. 1995, 84, 1193.
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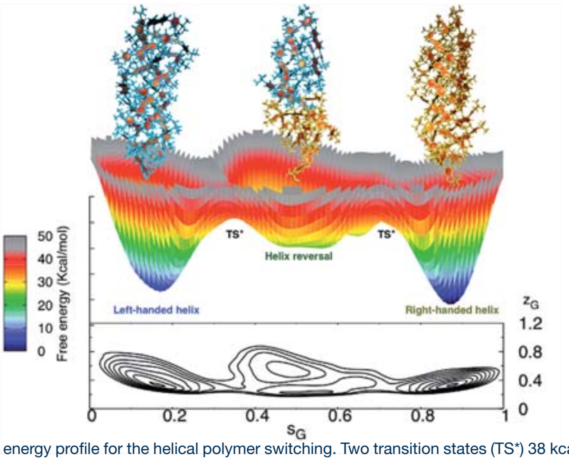

Free energy profile for the helical polymer switching. Two transition states (TS*) 38 kcal/mol higher connect the Left- and Right-handed basins. A broad minimum in between identifies the helix reversal state.[3]

Large-eddy simulation on unstructured meshes for internal combustion engines

Federico Piscaglia
Politecnico di Milano

The dynamics and evolution of turbulent structures inside an engine-like geometry are investigated by means of Large Eddy Simulation. A simplified configuration consisting of a flat-top cylinder head with a fixed, axis-centered valve and low-speed piston has been reproduced in the finite volume code OpenFOAM. The standard version of the software has been extended by the authors with enhanced capabilities, including topologically changing grids, mesh handling of non-conformal interfaces, advanced SGS models and boundary conditions for LES simulation. Parallel algorithms for data post-processing have been also developed. The developed software is able to run both on BGQ and PLX architectures. Part of the work has been also used by a joint collaboration between Cineca and the investigators within the PRACE framework.

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(3) F. Piscaglia, A. Montorfano, and A. Onorati, “Development of fully-automatic parallel algorithms for mesh handling in the openfoam-2.2.x technology,” SAE paper 2013-24-0027.
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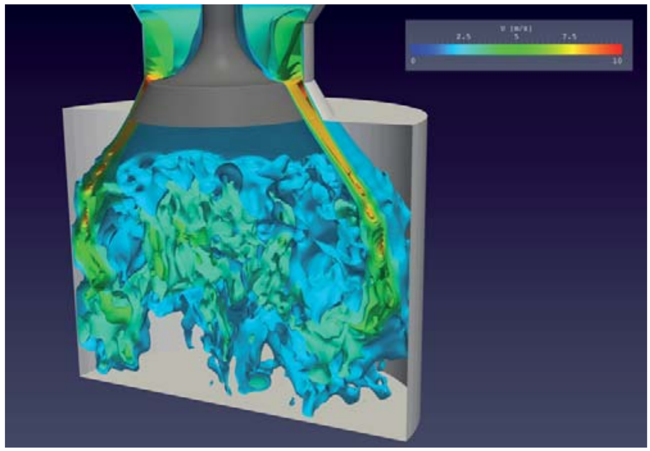
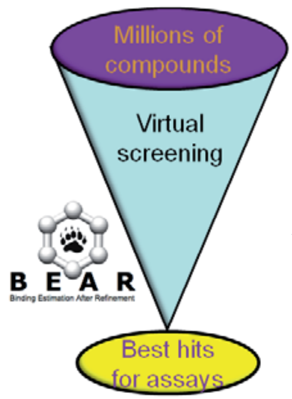


Snapshot of isosurfaces of velocity inside the cylinder at crank-angle 85° after Top Dead Center on cycle 2. Surfaces are colored according to velocity magnitude

BEAR (Binding Estimation After Refinement), a powerful tool for virtual screening of potential drugs

Giulio Rastelli
Modena and Reggio Emilia University

In the drug discovery process, accurate computational methods for predicting the biological activity of small molecules towards a desired biological target are urgently needed. The Molecular Modelling & Drug Design Lab at the University of Modena and Reggio Emilia has set up and validated an innovative computational technology named BEAR (Binding Estimation After Refinement), which has proven to perform significantly better than commonly used virtual screening methods. BEAR is an automated post-docking procedure for the conformational refinement of docking poses through molecular dynamics followed by accurate prediction of ligand binding free energies using MM-PBSA and MM-GBSA.
In our computing initiative, we have exploited our virtual screening technology on a high performance computing platform at Cineca to efficiently screen new potential ligands with a potential to become anticancer drugs. The possibility of running BEAR on large scale computing infrastructures such as SP6 has made it possible to screen in silico millions of compounds on multiple drug targets.



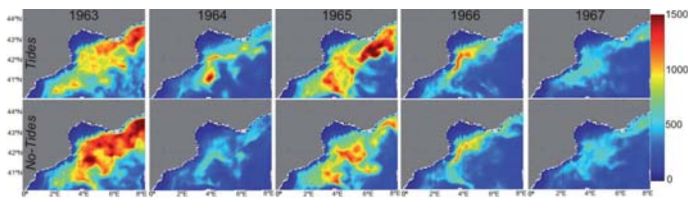
Virtual screening of large databases of chemical compounds in the binding site of a drug target allows the rational identification of a smaller set of best hits to be submitted to biological and pharmacological assays.

Evaluating the effects produced by tides on mthc

Gianmaria Sannino
ENEA

The Mediterranean Thermohaline Circulation (MTHC) is mainly sustained by the atmospheric forcing and controlled by the narrow and shallow Strait of Gibraltar (hereinafter SoG). Within the SoG the MTHC takes the form of a two-way exchange. The interaction between the intense tidal forcing and the complex geometry of the SoG influences the two-way exchange via hydraulic control. Despite the key role played by the SoG, none of the ocean models implemented recently for the Mediterranean was able to fully simulate the Strait dynamics. The main limiting factors were the coarse resolution adopted for the Strait and the omission of tidal forcing. Thanks to the resources provided by ISCRA we have overcome these limitations by implementing an innovative Mediterranean tidal circulation baroclinic model (MITgcm) characterized by a non-uniform horizontal curvilinear grid that reaches the resolution of 1/200° in the Strait and degrades inside the basin to 1/16°. We have evaluated the effects played by the SoG dynamics, and tides on the simulated MTHC by comparing results from two simulations, ten years long, forced with and without tides respectively. The comparison revealed that the tidal simulation represents correctly the two-way exchange.

Moreover, while the main characteristics of MTHC are similar in the two simulations, some significant differences are evident: a residual barotropic velocities is observed, as well as an impact on the water stratification throughout the basin affecting the large scale properties as for example the mixed layer depth in the Gulf of Lion.



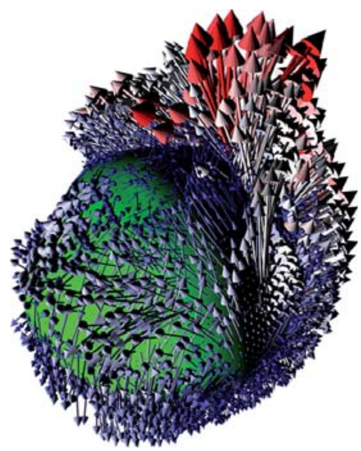
Mean Mixed Layer Depth in the Gulf of Lion computed for different years with the Tides simulation (upper panel) and the No-Tides simulation (lower panel).

Dispersion of Particles in Stratified Turbulence

Alfredo Soldati
Udine University

Many geophysical flows, such as in the oceans, lakes or atmosphere, are influenced by the presence of stable stratification: the ability to predict mixing and dispersion in these situations is therefore of great importance. In unstratified turbulence, particles can move vertically (over unlimited distances) under the influence of vortical structures. In stably stratified turbulence, work must be done against buoyancy to move particles in the vertical direction and particle dispersion is strongly modified. The fundamental physics of the above mentioned processes is just partially understood, and much more remains to be learned.

In this project we proposed a systematic study of the interaction between stratified turbulence and particle dispersion/deposition in free surface flows. We used high-resolution pseudo-spectral Direct Numerical Simulations (DNS) for the solution of the Navier-Stokes equations and Lagrangian Particle Tracking (LPT) for the analysis of particle dynamics. Our results showed that modification of turbulence due to thermal stratification strongly influences particle dispersion in the bulk of the flow. At the free surface, stratification effects are also observed on the clustering of particles: the filamentary particle patterns observed in unstratified turbulence are progressively lost as thermal stratification increases, and particle distribution remains roughly two-dimensional.

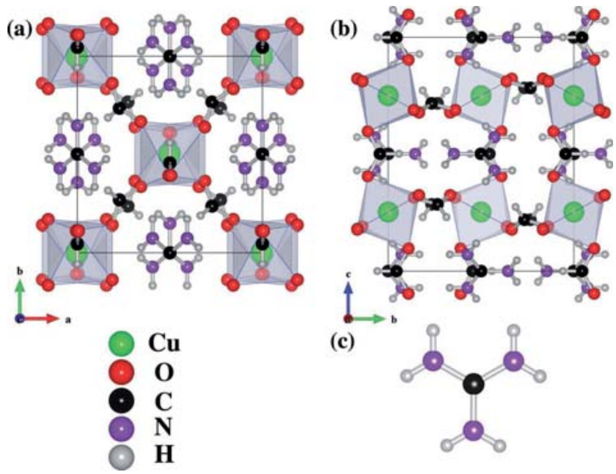


Vector plot of the velocity fluctuations over the interface of the droplet (in green); high turbulence regions are shown in red, whereas low turbulence regions are shown in blue.

Hybrid Improper Ferroelectricity in a Multiferroic and Magnetoelectric Metal-Organic Framework

Alessandro Stroppa
CNR-SPIN

On the basis of first-principles calculations, we design a novel Cr-based metal-organic framework to be both multiferroic and magnetoelectric. The compound shows a “double-hybrid” nature: it is a hybrid organic-inorganic compound and it shows hybrid improper ferroelectricity. Here, the coupling of non-polar distortions, such as Jahn-Teller pseudo-rotations and tilting, pave the way to a polar behavior, with the coupling being realized through hydrogen bonds.



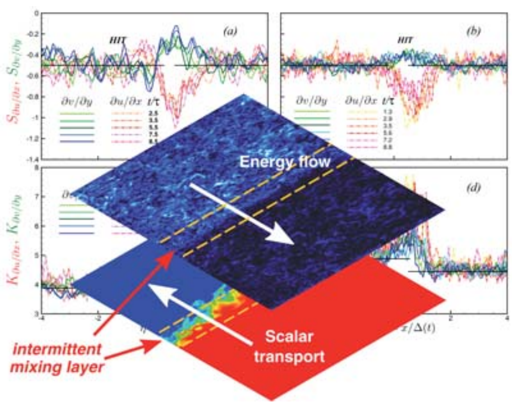
(a) top and (b) side view of the crystalline unit cell; (c) Guanidinium cation.

Turbulence mixing and small scale anisotropy

Daniela Tordella
Politecnico di Torino

Two sets of numerical experiments have been carried out to study the generation of small-scale anisotropy from the interaction between two decaying isotropic turbulent flows with different statistics in absence of a mean shear. The inhomogeneity is due to the presence of a kinetic energy gradient or a spatial perturbation of the correlation length. This inhomogeneity produces a highly intermittent mixing layer between the two homogeneous regions. The transport of a passive scalar across the mixing is considered.

The main result is that the mixing produces a compression of the flow filaments lying across the mixing layer and an extension of those in the normal directions. The structure of the small scale anisotropy follows a pattern where the odd moments of the transversal velocity derivative are negligible while the moments of the longitudinal velocity derivative moments significantly vary in the direction normal and parallel to the mixing. This pattern is different from the anisotropy created by a mean shear, which produces high transversal derivative moments but has little impact on longitudinal derivatives. When initially uniform kinetic energy, an inhomogeneous integral scale produces different decay rates of the kinetic energy in the two homogeneous regions with a transient phase during which a kinetic energy gradient is generated. It has a lifetime roughly proportional to the integral scale ratio between the two regions.

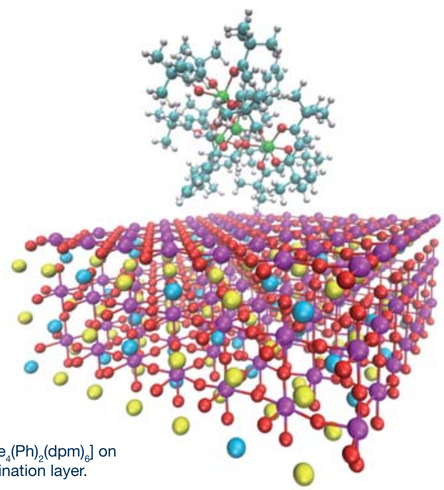


Scheme of the flow showing the interaction between two homogeneous and isotropic turbulent flows and the resulting kinetic energy and passive scalar transport. In the background the longitudinal derivative velocity moments are shown (PRL 2011, Physica D 2012).

A step forward to future devices: DFT simulations of SMM on Manganites

Federico Totti
Florence University

This Project addressed, from the theoretical sides, radically new nanostructured materials for spintronics based on hybrid organic-inorganic architectures and containing Single-Molecule Magnets (SMMs) as active components. In this work we have used the SMM $[Fe_4(Ph)_2(dpm)_6]$, (Hdpm = dipivaloylmethane). SMMs are magnetically-bistable molecules displaying a memory effect at low temperature discovered in the early 90s. The results obtained are propaedeutic to the understanding how an electric current driven through a SMM can control and sense the large molecular magnetic moment. In this framework this project helped to elucidate the microscopic interaction between deposited SMMs and the underlying the FM substrate, in this work $[La_{0.76}Sr_{0.33}MnO_3]$, LSMO. The periodic DFT calculations where performed in framework of the Gaussian and Plane Waves (GPW) formalism.
Indeed, the Project shed lights on the extent of changes, with respect to the isolated components, occurred in the relevant properties of both systems when interfaced. In particular, our analysis focused on: 1) structural properties (in terms of bond lengths, bond angles, distortions etc); 2) electronic properties (in terms of density of states, core levels, charge densities, etc); 3) magnetic properties (in terms of exchange constants, magnetic moments, spin density, magnetic anisotropy energies etc).

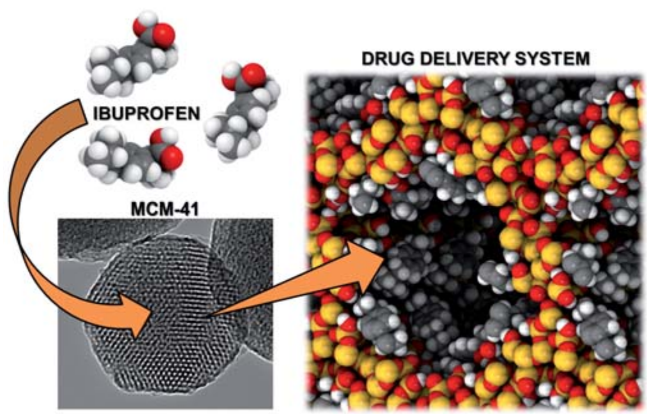


Optimized geometry of $[Fe_4(Ph)_2(dpm)_6]$ on LSMO with a $[MnO_2]$ termination layer.

Quantum mechanical modeling of the interaction of ibuprofen with the mesoporous MCM-41 material

Piero Ugliengo
Chemistry Department, Torino University

The interest in the pharmaceutical employment of amorphous silica has rapidly grown in recent years following the development of silica-based mesoporous ordered materials and the discovery of their biomedical applications. Among silica-based mesoporous materials, MCM-41 is one of the most studied since it was proposed as a drug delivery system. Notwithstanding the relevance of this topic, the atomistic details about the specific interactions between the MCM-41 surfaces and drugs and the energetic of adsorption are almost unknown.
We resort to Density Functional Theory (DFT), to simulate the features of the MCM-41 mesoporous silica material with respect to adsorption of the ibuprofen drug. We sampled the potential energy surface of the drug-silica system by docking the ibuprofen molecule on different spots on the pore walls of a realistic MCM-41 model. The drug loading was gradually increased towards an almost complete surface coverage. Ab-initio molecular dynamics simulations was also performed to investigate the drug mobility.
Our results show that ibuprofen adsorption is an exothermic process following a quasi-Langmuirian model. Noteworthy, dispersion (vdW) interactions were playing a crucial role in dictating the features of the drug/silica system. Simulations of IR and NMR spectra provided useful information to interpret ambiguous experimental data.



Ibuprofen drug, transmission electron microscopy of MCM-41 (C.T. Kresge et al, Nature 1992, 359, 710) and ibuprofen interacting with the internal walls of a MCM-41 in silico model.

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