CINECA

Cineca HPC Report 2016
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ISBN 978-88-86037-35-8

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Thanks to:
Fabio Affinito, Chira Aieta, Paola Alberigo, Matteo Amabili, Michela Arnaboldi, Giulio Barcaroli, Sanzio Bassini, Ugo Becciani, Matteo Bernardini, Luca Biferale, Fabio Bonaccorso, Francesco Califano, Luigi Calori, Lorenzo Casalino, Carlo Massimo Casciola, Tommaso Cavallucci, Carlo Cavazzoni, Michele Ceotto, Alberto Debernardi, Andrew Emerson, Giovanni Erbacci, Mauro Felicori, Giuseppe Fiameni, Luca Franci, Daniel Fuster, Fabio Gabas, Daniela Galetti, Chiara Galletti, Alberto Giacomello, Leonardo Giusti, Massimiliano Guarrasi, Antonella Guidazzoli, Petr Hellinger, Khatuna Kakhiani, Simone Landi, Simone Landi, Yue Ling, Emanuele Lisi, Alessandra Magistrato, Gian Franco Marras, Lorenzo Matteini, Simone Meloni, Silvia Monfardini, Paolo Orlandi, Giulia Palermo, Eric Pascolo, Antonino Petralia, Francesco Pierantoni, Sergio Pirozzoli, François Rincon, Alessio Roccon, Elda Rossi, Ursula Rothlisberger, Marco Scarnò, Alexander A. Schekochihin, Gabriella Scipione, Donatella Sforzini, Alfredo Soldati, Nicola Spallanzani, Stefano Tarsi, Valentina Tozzini, Claudia Truini, Grétar Tryggvason, Roberta Turra, Francesco Valentini, Alberto Vecchiato, Andrea Verdini, Roberto Verzicco, Stephane Zaleski, Francesco Zonta.

Cineca HPC Report

2016

Dear Colleagues,

In continuity with a consolidated tradition, I am very pleased to present the Cineca HPC Report of the achievements and outcomes obtained during the year 2016. In the aim of a persistent commitment about our effort in High Performance Computing and its correlated activities, as big data management and processing, high throughput, urgent and cloud computing, the year 2016 has been a very important keystone in the development process of Cineca.

The main occurrence has been the introduction of a new tier 0 HPC system in production. I am referring to the installation of the two first partitions of the Marconi system that replaced the previous Fermi system introduced in production in the past 2012. Confirming our ambitious and temporally short cycle frame of innovation process, as in the long tradition of Cineca in the order of 36 / 40 months, not more, a new project structured in two steps, replacement of Fermi with a new supercomputer having a computing power order 10x respect its predecessor for a cycle of three years, and than a following phase having 10x more computing power, was approved by Cineca governance with an investment as whole of 50 Millions of Euro. In the 2017 the Marconi project will be completed with the installation and inclusion in production of the third partition of the system that will bring the whole performance of the Marconi system in the order of 20 PF peak, meet the main objective of the project. As detailed in this report, the Marconi supercomputing system is designed as a flexible single system image supercomputing platform, which combines conventional and non conventional microprocessors technology, in the aim to optimize the energy efficiency of the whole architecture according to ours open shop workload.

As in the past the access to the system will be based on the scientific merit by mean of open access peer reviewed process, managed by PRACE at International European level, and ISCRA at National level. The service will be also open to the community of few qualified organizations as Eurofusion, for which Cineca will act as main HPC providers, National Research Agencies, Infrastructural projects funded by the European Commission. The emerging of the data driven paradigm, the forth one method aside with theoretical, experimental and computational, to progress in scientific research and innovation pose the rational for an increasing attention in the valorizations of and ecosystem of competences, beyond the vertical competences in computational methodology. In a wide spectrum of know how ranging from bioinformatics to visualization and computer graphics, from data analytics to cognitive computing. That pose the large scale digital infrastructure for the computing and big data processing at the center of disciplinary domains as cultural heritage, multimedia technology, sentiment analysis that are of increasing importance in the processes of decision support. Of those contexts, details and documentations is included in the report to remark that important outcomes were achieved also for such applications domains, clearly, thanks to our very skilled staff, one of the main asset of Cineca, and by mean of a strong cooperation with our researchers and scientists, as well as, of course, the strong support ensured by our funding agencies, to whom we will continue demonstrating the value of keeping Italian digital infrastructure at the top level of the international panorama.

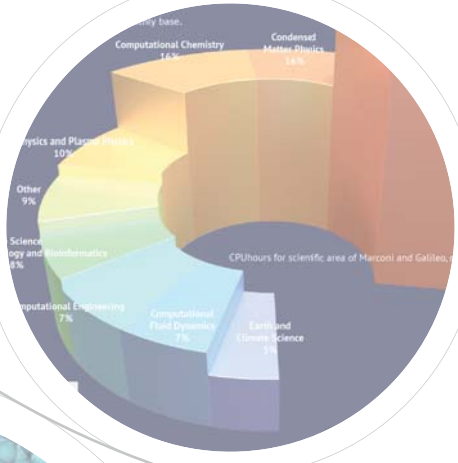
With kindest regards,

Sanzio Bassini

Director of SuperComputing Applications and Innovation Department of Cineca

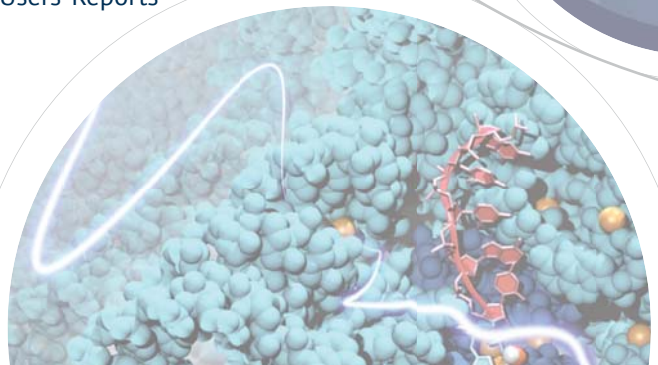
Section 1: MARCONI

Section 2: National&international collaborations



Section 3: 2016 HPC in numbers, assessment and impact

Section 4: Scientific Reports



HPC Evolution in Cineca

Computational applications integrated with extreme data applications are gaining traction in science and industry and big data analytics as a whole is growing in importance by providing unprecedented and intuitive insights in science but also in business, economic and social fields.

Future large-scale simulations running on the new pre-exascale supercomputers will become more and more data-intensive and require an integrated data and HPC infrastructure.

New HPC & data oriented infrastructures, supporting open science policies, would become soon a valuable asset for the scientists.

Cineca, in its mission of supporting the Italian and European research community to accelerate the scientific discovery - using HPC resources in a profitable way and exploiting the newest technological advances in HPC and data management – is conscious of this change of paradigm.

The Cineca compute-centric infrastructure is making a step forward in the realization of a Data Centric infrastructure, where data covers a fundamental role in any scientific application. In our view, the transition from a silos centric organization (where different computing platforms rarely interact together) towards a more integrated data oriented environment (where various types of workloads are supported and data can be accessed from all computing engines efficiently) represents an important breakthrough with respect to the past.

In 2016, MARCONI, the new Tier-0 system replaced FERMI, increasing the performance from 2 PFlop/s to a performance in excess of 12 PFlop/s (in the first stage), and reaching a 10 million-fold increase in performance for the Cineca's HPC systems since 1993, when the TOP500 classification started. In this long period, Cineca has been always able to fully exploit at the evolution of the architectural paradigms, for the benefit of the Italian scientific community.

MARCONI is planned in two technological stages in a 5-year program, with the objective to reach a 50 PFlop/s system by the year 2019-2020. The first stage, composed of 3 different partitions, started in April 2016 with the installation of the Broadwell partition (2PFlop/s). The second partition was installed in October 2016 (10PFlop/s KNL system, ranked N. 12 in the TOP500 list - November 2016). In mid 2017 the third partition (Sky-lake system) will complete the first stage.

Then, in 2019, the MARCONI system will evolve to reach a global performance of 50 PFlop/s, integrating the HPC and the data infrastructure, thanks to the fore-coming innovation in the field of new memory technologies.

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

The size and resolution of the problems scientists will address are limited only by the size of the data they can reasonably work with. There is a constantly increasing demand for faster processing on bigger data.

The architectural plan for the second stage MARCONI in 2019 will support the convergence of data and HPC technologies, fundamental to facilitate the integration of scientific methodologies with advanced usage models and methods required to burst new workloads i.e. the ones represented by machine learning and cognitive computing.

The innovative architecture of the Tier-0 MARCONI system and its evolution in the time-frame 2016-2020, together with the availability of significantly larger computational resources, will represent a further step ahead for Italian and European scientists to reach new scientific breakthroughs.

Furthermore, with Marconi, Cineca significantly contributes to the growth of the European HPC Ecosystem being a pillar of the PRACE HPC infrastructure, being one of the four building blocks of the High-Performance Analytics and Computing Platform in Human Brain Project, and by hosting the system dedicated to the fusion research in Europe (EuroFusion): a combined system providing a performance of one PFlop/s standard CPUs and one PFlop/s accelerated by the end of 2016, that will be upgraded to 5 PFlop/s standard CPUs and one PFlop/s accelerated in 2017.

Giovanni Erbacci
Cineca

MARCONI: a new supercomputer at Cineca for Italian and European research community

Marconi is the new Tier-0 system, co-designed by Cineca and based on the Lenovo NeXtScale platform, that substitutes the former IBM BG/Q system (FERMI). MARCONI is based on the most recent generation of the Intel® Xeon product family, putting together more traditional chips (Intel® Xeon® processor E5-2600 v4 product family – Broadwell and then Skylake) alongside with the new many-core chips (Intel® Xeon® Phi – codename Knights Landing). The aim is to offer the scientific community a technologically advanced and energy-efficient high performance computing system.

This achievement represents the first step of the Italian infrastructure development plan put forward by Cineca, aimed at supporting scientific research. The global plan entails an investment of Euro 50 million in two phases. The first, started this year, will make available a computational power of about 20Pflop/s and a data storage capacity of more than 20 Petabytes, which will go into production, reaching completion in the second half of 2017. The second phase will start during 2019, with a final goal to increase available computing power to approximately 50 to 60 Pflop/s by 2020.

The new system, logically named 'MARCONI', will gradually be completed in about 12 months, between April 2016 and July 2017, according to a plan based on a series of updates:

• A1: This preliminary system went into production in July 2016, based on Intel® Xeon® processor E5-2600 v4 product family (Broadwell) with a computational power of 2Pflop/s.

• A2: by the end of 2016 a new section is being added, equipped with the next-generation of the Intel Xeon Phi product family (Knights Landing), based on a many-core architecture, enabling an overall configuration of about 250 thousand cores with expected additional computational power of approximately 11Pflop/s.

• A3: finally, in July 2017, this system is planned to reach a total computational power of about 20Pflop/s utilizing future generation Intel Xeon processors (Sky Lake).

This supercomputer takes advantage of the new Intel® Omni-Path Architecture, which provides the high performance interconnectivity required to efficiently scale the system's thousands of servers.

A high-performance Lenovo GSS storage subsystem, that integrates the IBM Spectrum Scale™ (GPFS) file system, is connected to the Intel Omni-Path fabric and provides data storage capacity.

The progressive development of the Marconi system will allow use of state-of-the-art processor technology, enabling an extremely high-performance system but still with a 'green' soul. One of the parameters of the project developed by the Cineca team is in fact to gradually increase the computational power up to 50Pflop/s without exceeding, at any stage, the limit of 3MWatt power consumption.

MARCONI Broadwell was first ranked in TOP500 in June 2016 and reached the position 46 with a sustained performance of about 1.7 Pflops. In the most recent TOP500 list, announced Monday, November 14, at the SC16 conference in Salt Lake City, Utah, the second upgrade (MARCONI Intel Xeon Phi) was ranked number 12, reporting a sustained performance of about 6.2 Pflops.

The MARCONI computing system installed at Cineca in Autumn 2016 is the largest supercomputer available in Italy today, and also the number one among the European Community Countries, as far as the scientific computing systems are considered. This second upgrade of MARCONI brings Italy among the Countries delivering a high level of National HPC power, just after: China, United States, Japan, Germany, Great Britain and France.

Elda Rossi
Cineca

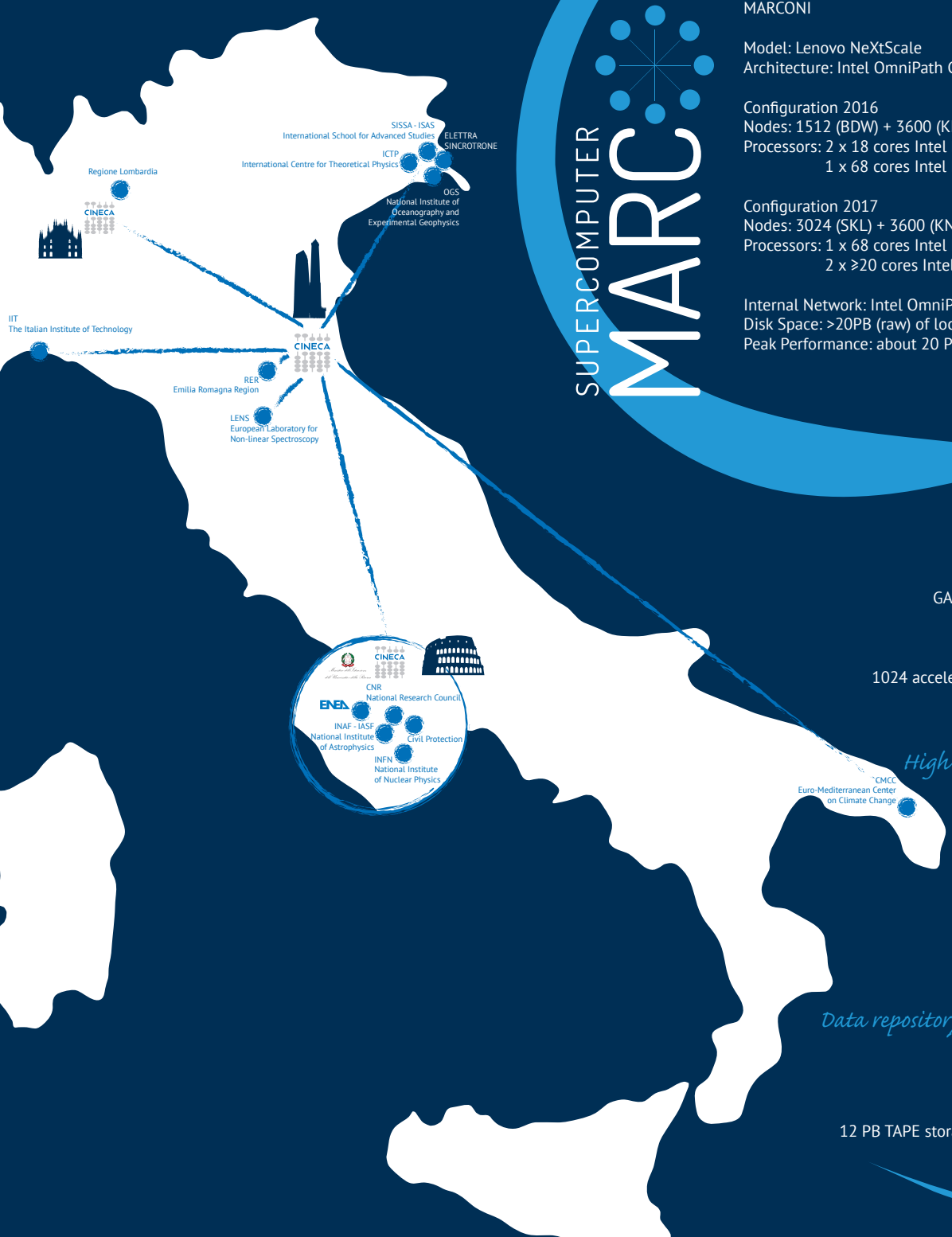
SUPERCOMPUTER
MARCONI
"Every day sees humanity more victorious in the struggle with space and time."
Guglielmo Marconi
CINECA
lenovo

MARCONI: a multi step HPC Cineca project unity

The implementation of MARCONI project is planned in three phases, each one characterized by a portion of the cluster with a specific processor and a specific cooling solution. Against the fact that the power consumption of the three portions of the cluster are quite similar, the cooling method adopted for each part is very different, due to the different processors types and their density on the chip.
The first phase, called A1 part, without accelerators, could be cooled with air or with water. In order to evaluate the best solution, analysis and simulations have been carried out in collaboration with the researchers of the University of Bologna.
The results of the comparison of the different scenarios showed that the air cooling system was enough with racks arranged in two rows, with large space between and active floor. That means that under the grid between the two rows there are fans that push the cold air to give it more pressure reaching also the highest servers. The efficiency is increased by a confinement of the cluster inside a cage.
For the second phase, i.e. A2 part, that is more than double the A1 in terms of number of servers, with high density throughput optimized processors, a water cooling method has been adopted. The choice of the disposition of the racks seemed quite simple, because Cineca has only one water cooled machine room, that fits perfectly the required space floor.
So, you might think that part A2 was easier than part A1? Not at all.
A lot of suspense enfolded this period of the project, while the machine room needed to be completely refurbished and the work had to be done at a record speed to have chance to have a HPL result to publish in the TOP500 of november.
The power system was completely renewed, based for the first time in Cineca on busbars.
The pipes of the water cooling system have been totally substituted, to match the distribution of the new supercomputer. In fact the previous pipes system had been used to bring water to 10 large racks arranged in two rows on one side of the room, instead the A2 partition consists of 46 racks organized in 3 rows that completely fill the room. Other 4 racks of the A2 partition were previously placed in a different room, in the air cooling space close to the A1 partition, the Omnipath switches and the storage racks. The limited number of total servers of 4 racks allowed this choice of collocation and permitted to start working earlier with the new hardware and configurations and consequently to have a fraction of the cluster perfectly working before the water cooled room was ready to receive the rest of the A2 partition. This portion could be cloned to other 46 racks, as soon as they were placed in the refurbished computer room, saving a lot of time with the overlap of the installation activities. The success on this challenging part of the project arrived also thanks to a hard work and a strong and great coordination of all the teams involved in the installation.
The A3 part is expected in the first half of 2017. Also this partition needs water cooling, so further work needs to be done. While the water cooled room is already full of the MARCONI A2, a portion of the air cooled computer room hosting the A1 part has to be equipped with water cooling system.
The first step of this evolution had already been done, confining an area of the big room where the A1 partition is placed aside the Tier-1 and Tier-0 systems with a plexiglass wall.
In the meantime, the staff started to learn how to manage thousand of servers, early production processors, all connected with Omnipath (nickname OPA) network.

Daniela Galetti
Cineca

SUPERCOMPUTER MARCONI



New Tier-0

MARCONI

Model: Lenovo NeXtScale
Architecture: Intel OmniPath Cluster

Configuration 2016
Nodes: 1512 (BDW) + 3600 (KNL)
Processors: 2 x 18 cores Intel Broadwell @ 2.30 GHz, 54432 cores
1 x 68 cores Intel KnightsLanding @ 1.40 GHz, 244800 cores

Configuration 2017
Nodes: 3024 (SKL) + 3600 (KNL)
Processors: 1 x 68 cores Intel KnightsLanding @ 1.40 GHz, 244800 cores
2 x ⩾20 cores Intel SkyLake @ ~2 GHz, ⩾ 120960 cores

Internal Network: Intel OmniPath
Disk Space: >20PB (raw) of local storage
Peak Performance: about 20 PFlop/s

National Tier-1

GALILEO - IBM/Lenovo NeXtScale Cluster

512 nodes, Intel Haswell
8K cores
1024 accelerators (Intel Xeon Phi and nVidia K80)

High Performance Data Analytics

PICO - IBM NeXtScale Cluster

80 computing nodes
• thin/fat nodes 128/512 GB RAM
• hadoop and map reduce
• data insight
• remote visualization
• cloud computing

Data repository, curation and preservation

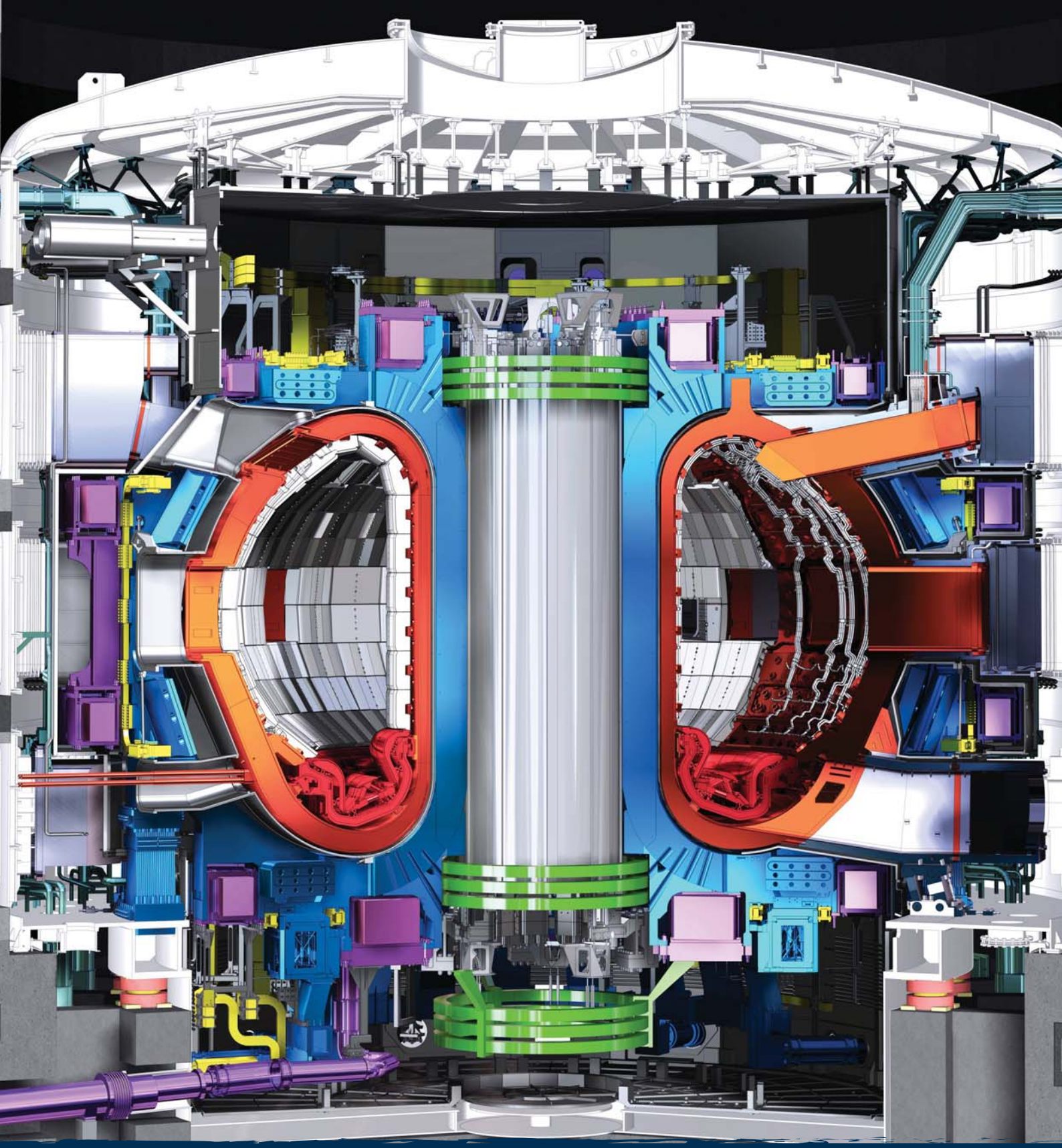
MULTI TIER STORAGE

40 TB fast (SSD) storage
5 PB GSS storage
12 PB TAPE storage, integrated with GSS through LTFS

EUROFUSION

Cineca, together with ENEA, as an all Italian partnership, succeeded in the international selection for supplying HPC and storage services to EUROFUSION, the European Consortium for research in the fusion energy.
The new supercomputer for the community, MARCONI-fusion, has been set up and put into production in the second part of 2016 and will remain available up to 2018. It is a partition of the new HPC cluster recently installed in Casalecchio di Reno (Bologna) and it takes the place of HELIOS, the previous platform hosted by the International Fusion Energy Centre in Rokkasho (Japan).
A large part of MARCONI (806 nodes out of 1512) are dedicated to EUROFUSION, corresponding to a computational power of 1 PFlops (10^12 Floating Point Operation per second). This infrastructure will be boosted in January 2017 with 1 more PFlop on the new "many core" cluster based on Intel KnightsLanding cpus, and will finally reach the complete delivery in July 2017 with other 5 Pflops on the 3d-phase MARCONI cluster based on next generation Intel cpus named SkyLake.
The kick-off event of the HPC service for EUROFUSION was in Bologna, in November 2016. The ENEA president (Federico Testa), the Director of Cineca (David Vannozzi), the Director of EUROFUSION (Tony Donnè) were present to the ceremony, as well as the Director of the nuclear department of ENEA (Aldo Pizzuto) and the Director of the HPC Department of Cineca (Sanzio Bassini).
HPC techniques are very important for researchers in the fusion energy field, in order to produce electric power from this source before mid-century. Very important is the computational modelling for plasma and materials, mainly to validate the experimental results obtained by the ITER reactor, as well as to design the next generation reactor DEMO. In the last few years, breakthrough advances convinced EUROFUSION to invest 30 Million euro each five years to renew the computing infrastructure dedicated to research.
EUROFUSION is the European Consortium for research on fusion energy. 29 Institution in 27 different Countries are part of the consortium that was constituted in 2014 as a funding agency on behalf of Euratom.
ENEA is the Italian National Agency for emerging technologies, energy and sustainable economic development, made of 9 research sites around Italy and about 2.600 employees.

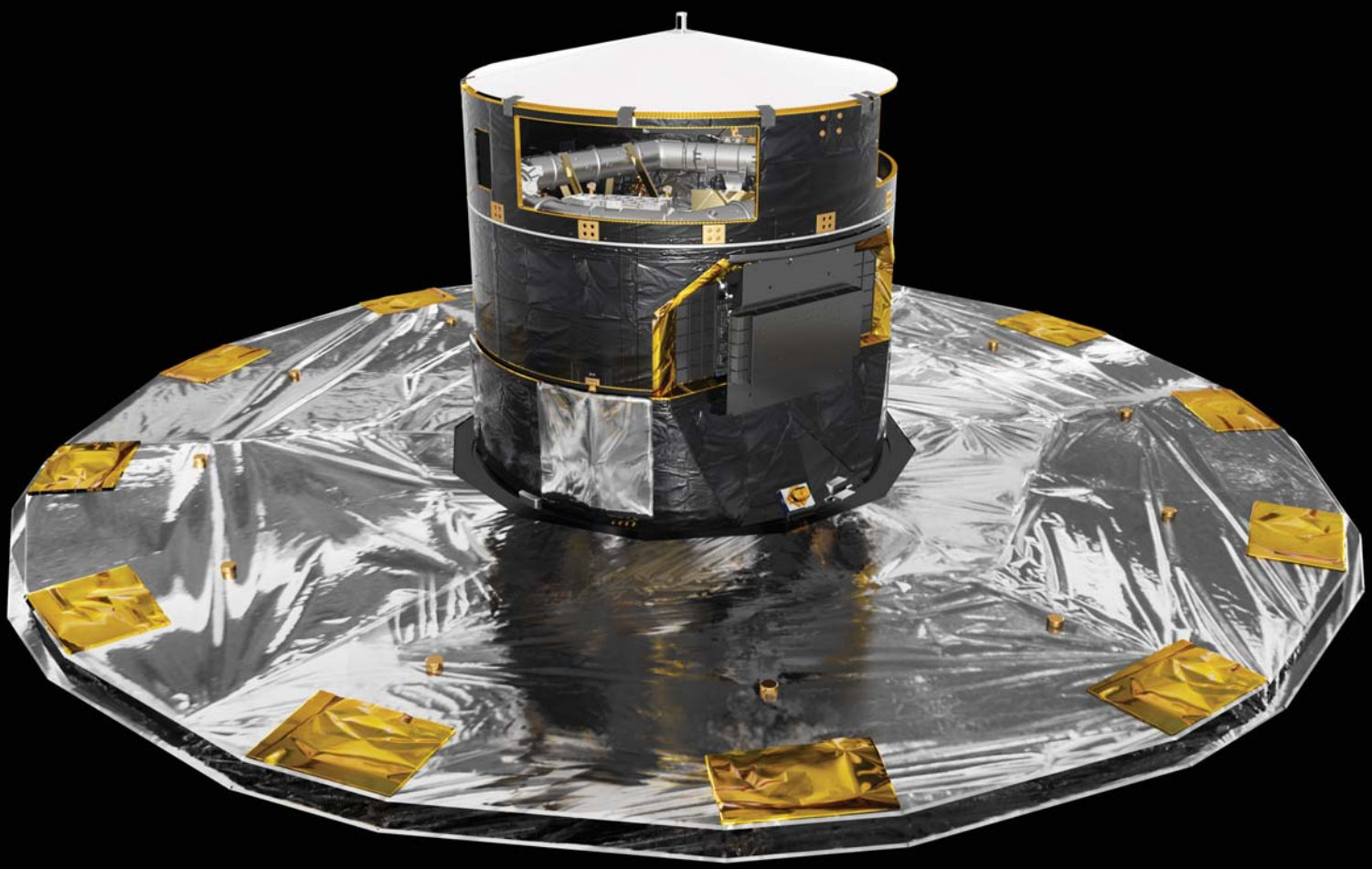
Elda Rossi
Cineca



The ITER TOKAMAK is being built in Cadarache (FR)

GAIA Mission & Cineca

The collaboration between the Italian astrophysics community and Cineca started many years ago, when the supercomputers started to be used to solve cosmological problems. Since then the availability of state of the art supercomputers and properly designed scientific codes, become more and more important for theoretical astrophysics. Nowadays it is possible to simulate stars, galaxies, and the whole universe with an accuracy that allows researchers to obtain quantitative comparison with cosmological observations.
For those reasons INAF (Italian national institute for astrophysics) has signed an agreement with Cineca to collaborate in delivering the best HPC infrastructure and the best competence in HPC software development to help the Italian astrophysics community to be competitive with other international research organization of the field.
The collaboration includes the access to the flagship Cineca HPC system (Marconi) for the researchers involved in INAF key projects, and the setup of a team of people (Cineca and INAF) with cross competence (HPC and Astrophysics), to enable applications for massively parallel computations.
The agreement between Cineca and INAF foresee also the possibility to extend the benefits of the access service and high level support activities to other INAF research teams involved in international projects, not strictly related to the computational studies.
This is of particular relevance since in the last ten years the HPC infrastructures have been used, with an increasing importance, to support experimental or observative researches, mainly because of the activities related to the management and the analysis of large amount of data, for which standard departmental computational resources are largely inadequate.
This is the case of the support Cineca is giving to the INAF team involved in the GAIA space mission of the European Space Agency (ESA).
The main goal of the GAIA mission is the mapping of large subset (more than one billion) of all the stars of the Milky Way galaxy, with an accuracy never reached before. This includes the computation of the position and distances of all the stars in the subset based on the measurements made by the instruments installed on the GAIA spacecraft.
In fact, it is not possible to take a direct measurement of the distance between two stars,and they have to be derived from other type of measurements (typically a relative displacement of the star position with respect to very far objects as observed by the spacecraft in two different positions in space).
The derivation of the stars' position requires non trivial data processing, reductions and computations, which are under the responsibility of a consortium of scientific institution named DPAC (Data Processing and Analysis Consortium).
Within the DPAC consortium INAF researchers are responsible of the Global Sphere Reconstruction within the Astrometric Verification Unit (AVU/GSR) in the core processing activities, representing one of the two numerical techniques that will be adopted and confronted to derive the stars' position.
The GSR data are processed at the Italian Data Processing Centre (DPCT), which is constituted by ALTEC at Turin and Cineca. In particular, Cineca supports the team implementing the GSR with the infrastructure, and the consulting to develop and run a highly parallel code required to solve the system of equations relating all the parameters of the stars' observations, and finally derive an estimate of the star positions.
In particular, the GSR team and the Cineca support activities are organized in two phases: one for the development and testing of the parallel solution of the system of equations, and one for the processing of the real data coming from the spacecraft. In the first phase the focus is more on the software development, in the second phase more on guaranteeing the service quality to keep the pace with the progress of the space mission itself.



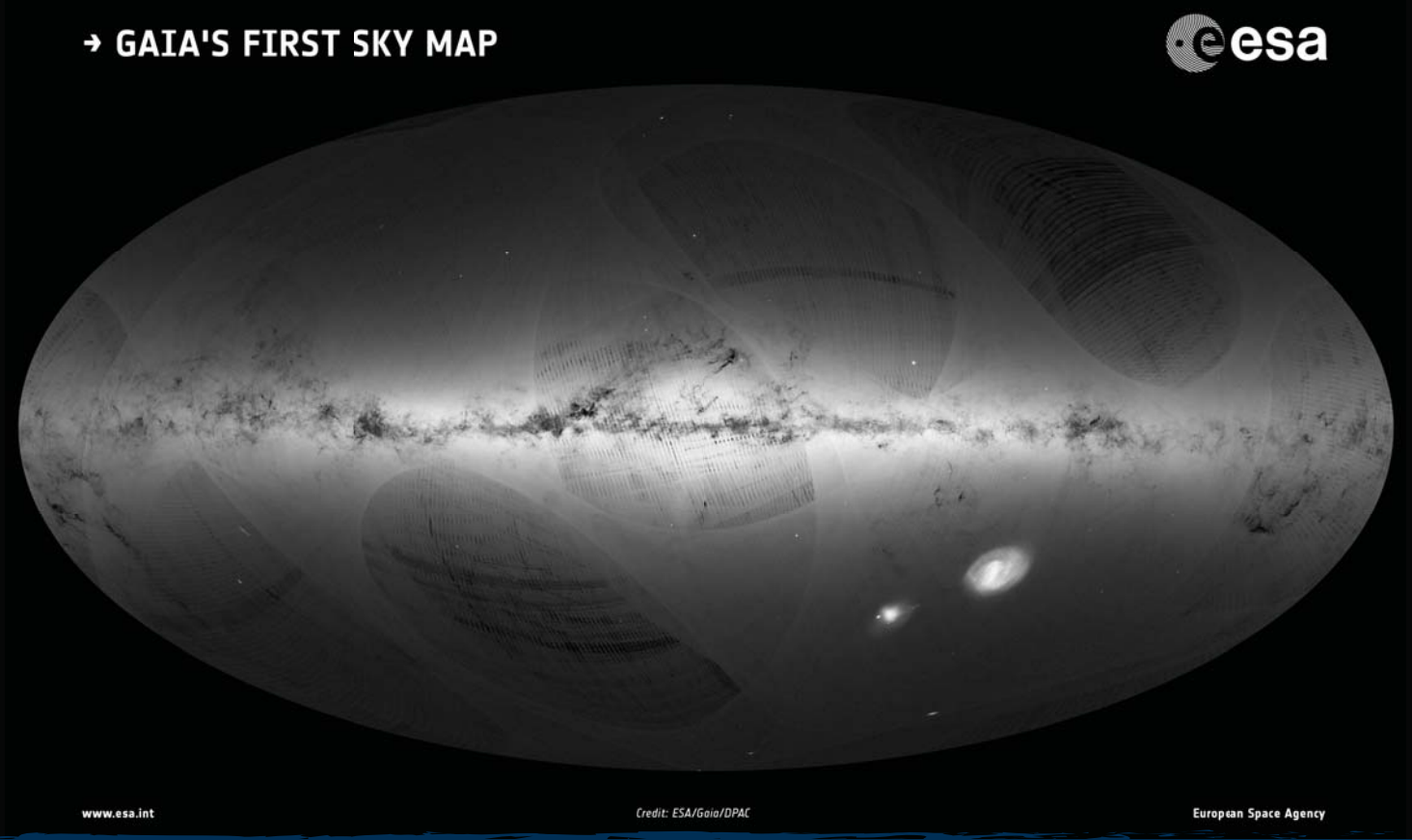
Artistic impression of the GAIA spacecraft (Credits: ESA/ATG medialab)

The activities for the GAIA mission involving the collaboration with Cineca will span over a period of time of about 10 years, being started in 2013. Roughly speaking 5 years to develop and testing the code and the data processing workflow (including the Cineca station), and 5 year of production.
The GAIA spacecraft installed on a Soyuz-Fregat vector has been launched in December 2013, and reached its final orbit (in the L2 point of the Sun-Earth system, about 1.5 million km from the Earth) in second half of 2014.
The GAIA mission will observe over one billion stars, and will compute the position of over 100 million of primary stars throughout the Milky Way.
The scientific researcher responsible for Italy of the GAIA mission is Dr. Mario G. Lattanzi, whereas the responsibility for the development of the part of the GSR workflow running at Cineca is shared between a team in the Observatory of Catania (resp. Dr. U. Becciani) and the Observatory of Turin (resp. Dr. A. Vecchiato).
The scientific and technical results, obtained within the scope of the collaboration will be shared between Cineca, INAF and ASI (Agenzia Spaziale Italiana). They can be disseminated, upon agreement, through scientific publications, technical reports, conferences and mass media to reach out a broader audience.

ESA mission official website http://sci.esa.int/gaia

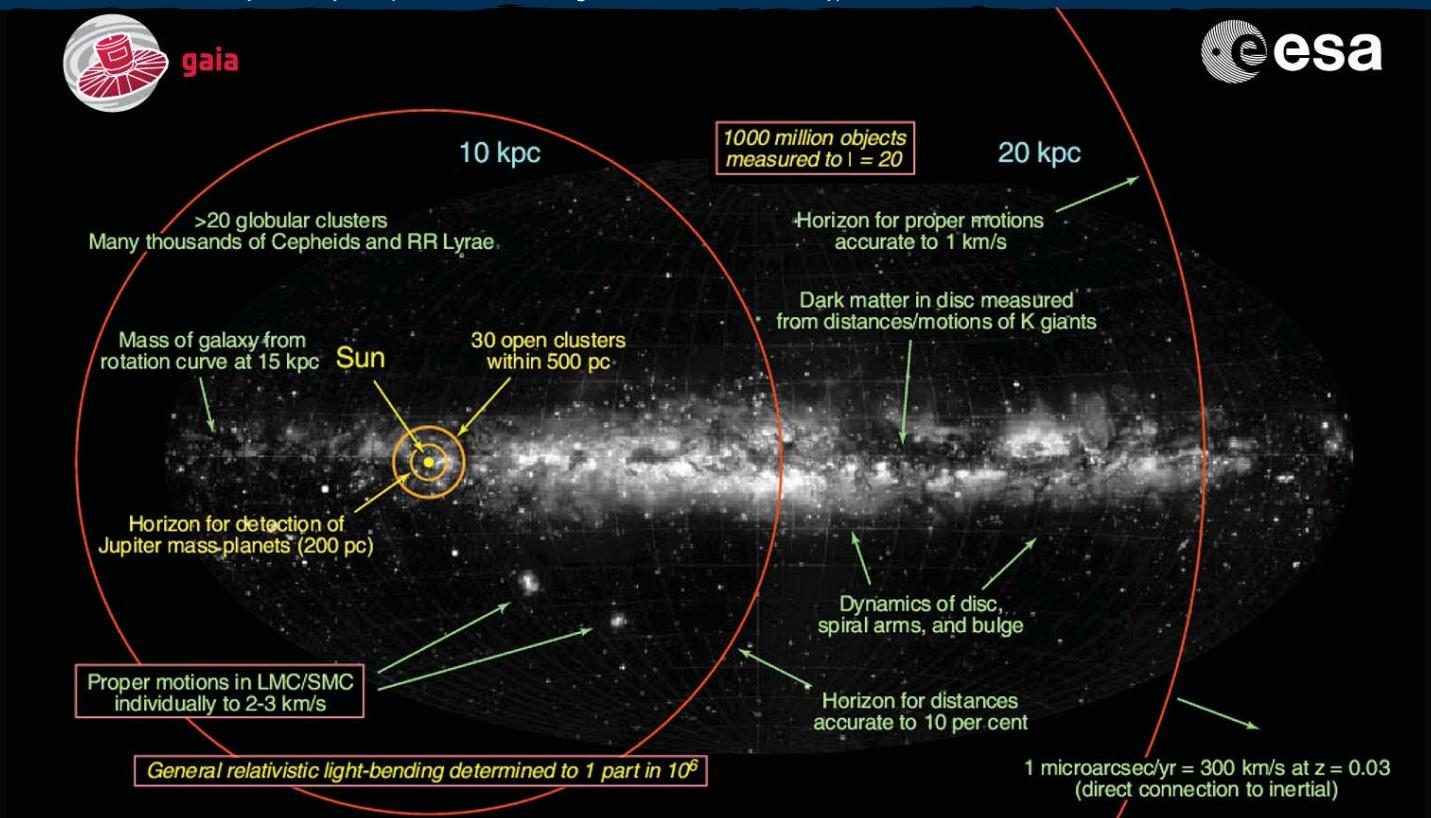
Carlo Cavazzoni
Cineca

Ugo Becciani, Alberto Vecchiato
INAF



Gaia's first sky map (Credits: ESA/Gaia/DPAC).

Gaia accuracies in the Galaxy and beyond (Credits: ESA, Background: Lund observatory).



Cineca and the weather forecasting service

Since September 1993, Arpae has been Cineca's closest partner in activities related to the national and navy weather forecast service. Cineca won several Community tenders for assignment of services and provision of supercomputing resources for predictive modeling weather and sea organized by Hydro-Climate-Weather service (Arpae-SIMC) of Arpae. Thanks to the collaboration with Cineca, OGS produces data on biogeochemical analyzes of the Mediterranean sea through the project "Copernicus: marine environment monitoring service", a service that provides information at European level on the quality of the sea and on the environmental conditions of seas and oceans skirting the continent. Through these partnerships, as well as with Arpae-SIMC and OGS, even with Arpa-Piedmont, CNR and others, Cineca has acquired many skills on predictive modeling both in meteorological and weather-marine who was in relation to the quality control air and seas.

Cineca can boast expertise in four distinct areas:

- management and administration of computational complex systems such as those of supercomputing;
- management of codes in supercomputing environment, parallelization, optimization and debugging;
- knowledge of predictive models regarding their configuration and their proper functioning;
- management of high criticality services in supercomputing environments.

In particular it has specific expertise on numerical techniques and parallelization of meteorological, climatological and oceanographic models. Many components of the COSMO, SWAN, Farm and many other models have been directly corrected and optimized by Cineca staff.

The service that is usually required in the weather - hydrological field, is coupling the typical problems of supercomputing systems with those of mission-critical services. The operation of a forecasting service that uses supercomputing must operate in unattended mode 365 days a year with strict deadlines and with an expectation of reliability and consistently high infallibility. To provide a service of this kind, each part of the infrastructure must be extremely reliable and redundant in its entirety and the environment must be stable over time and resist any critical event that can compromise its functionality.

The new contract significantly increases the demand for computing resources; now the various operative procedures have had an upgrade in terms of spatial resolution and coverage territorial.

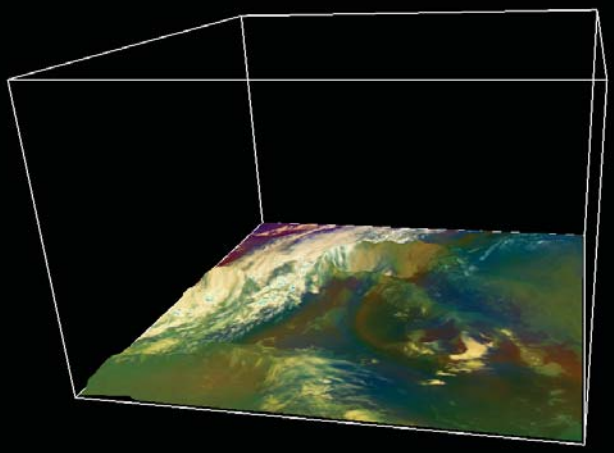
The procedure that handles the main weather prediction has passed from 7km as a spatial resolution on Italy to a 5Km with territorial coverage throughout the Mediterranean.

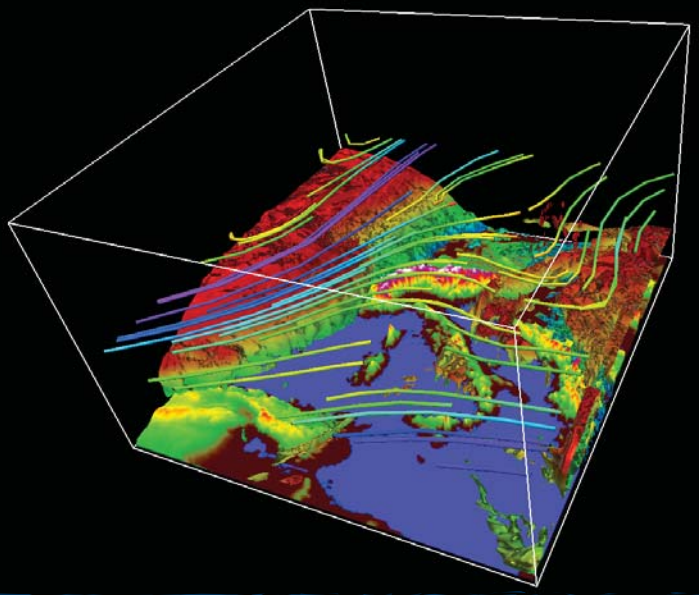
This upgrade requires an increase in computing resources 4 times higher.

Even the second forecast procedure has an increase of resolution from 2.8 to 2.2Km.

For the first time at Cineca by means of a probabilistic prediction ensemble forecasting techniques with a spatial resolution of 2.2 km and a new procedure for very short-term weather forecasting will also be activated.

Gian Franco Marras
Cineca

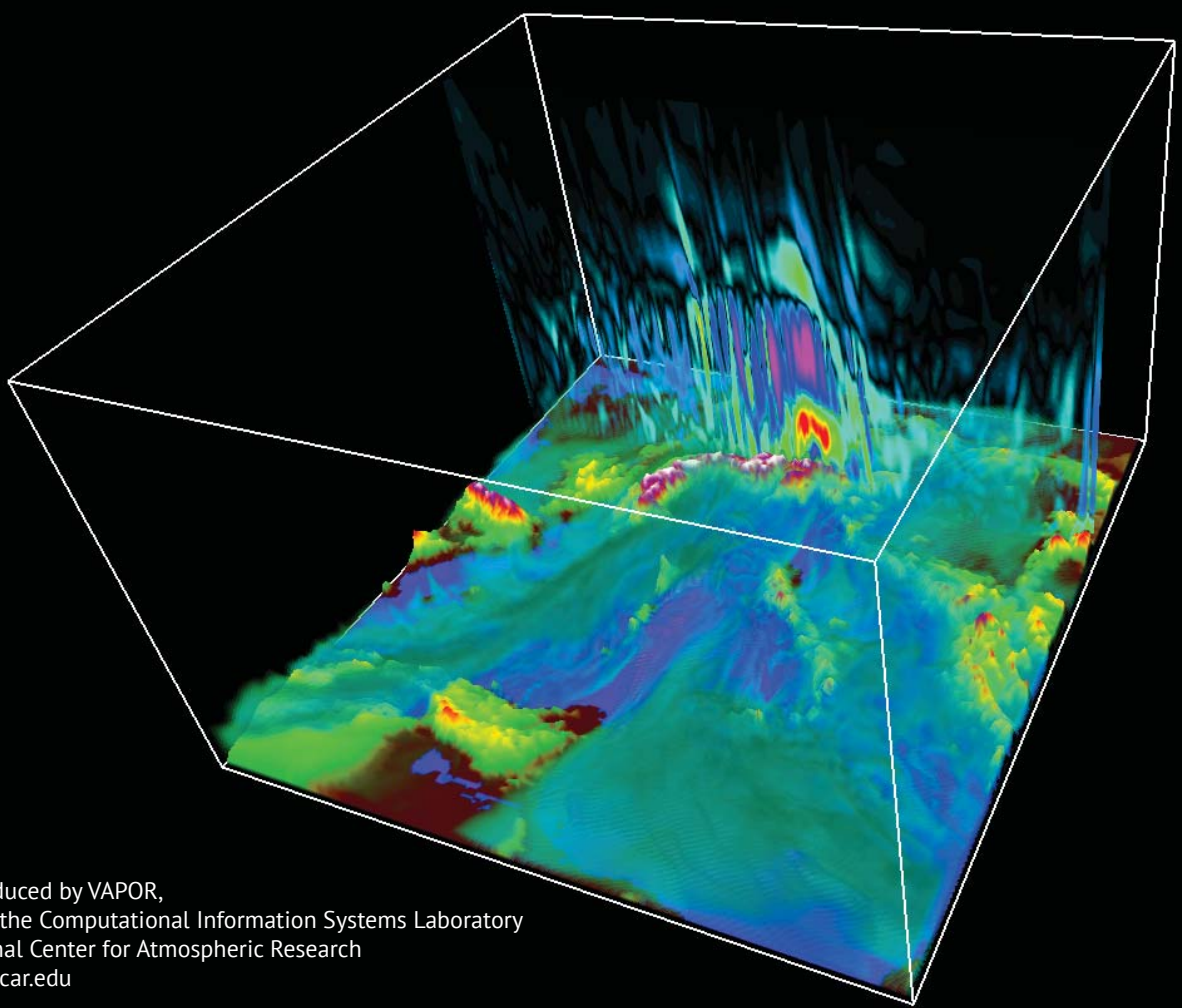




"air mass"_satellite processing

Isosurface pseudo-equivalent potential temperature, colored by temperature and streanlines

Cross session vertical velocity and volume rendering specific humidity



Imagery produced by VAPOR,
a product of the Computational Information Systems Laboratory
at the National Center for Atmospheric Research
www.vapor.ucar.edu

A Summer of HPC at CINECA

The PRACE Summer of HPC (SoHPC) is a outreach and training programme that offers undergraduate and junior postgraduate university students from all scientific disciplines the opportunity to spend two summer months at a HPC centre, in a PRACE partner country across Europe.

The programme aims to ensure a positive experience for all students and to encourage them in their path to become the next generation of researchers using HPC. The programme also aims to produce videos and visualisations to use in outreach activities and to generate interest in HPC and PRACE through social media.

Starting with a common training week on the HPC topics, the participants spend the months of July and August working on projects related to PRACE technical or industrial work and produce a report and a video of their results. Each participant has assigned a Project Mentor with whom he works closely on his project. Additional domain experts may be made available to work with participants. Flights, accommodation and a stipend is provided to all successful applicants.

At the end of the programme, the two participants which present the best results in the topics of visualisation and HPC outreach are awarded with respectively the Best Visualisation and the Best HPC Ambassador awards.

The Summer of HPC programme started in 2013 and since then Cineca participates to the initiative hosting two students every year. The edition 2016 of SoHPC has seen the application of 110 students from around Europe and 21 of them have been selected. Italy submitted 17 applications but only two Italian students have been admitted to SoHPC 2016.

After a kick-off training week at Juelich Supercomputing Centre attended by all participants, the students arrived to the 10 HPC PRACE centres involved in the programme. Cineca hosted two students from 4 July to 31 August 2016:

• Anurag Dogra, an Indian student with an undergraduate degree in Mechanical and Automotive engineering, now in the process of completing a master in Computational Material Science at TU Bergakadamie in Freiberg, Germany;

• Petr Valenta, from the Czech Republic, pursuing master's studies in Computational Physics at the Czech Technical University in Prague.

Petr worked to the project "In Situ or Batch VIsualization of biogeochemical state of the Mediterranean Sea", proposed by Paolo Lazzari from OGS, the National Institute of Oceanography and Experimental Geophysics, Trieste.

Anurag worked to the project "In Situ VIsualization of Navier-Stokes Tornado Effect", proposed by Prof. Sandro Frigio from the Universitiy of Camerino.

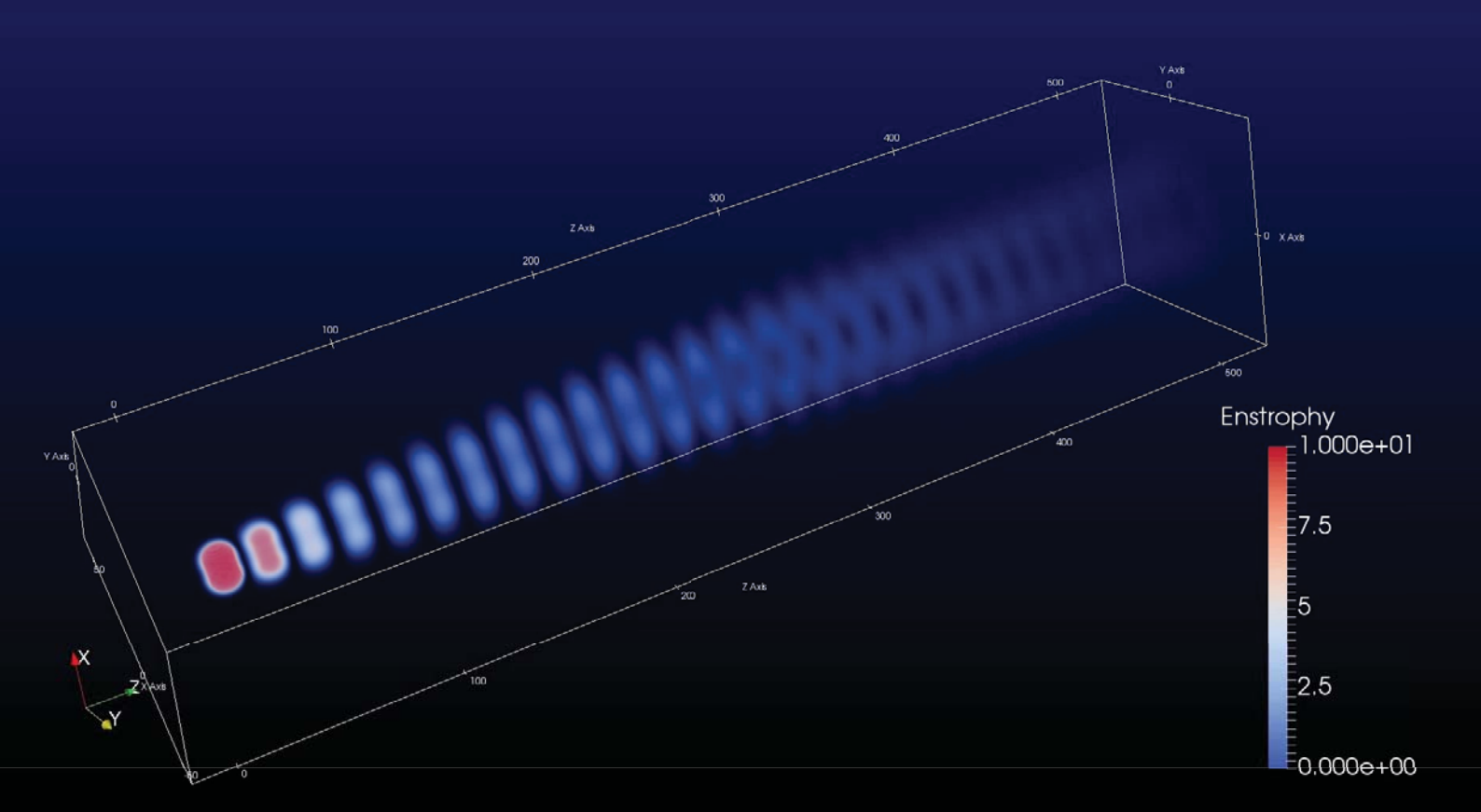
The students have been supported day by day by the Cineca SCAI mentors Massimiliano Guarrasi and Luigi Calori with the cooperation of the other experts in the SCAI team.

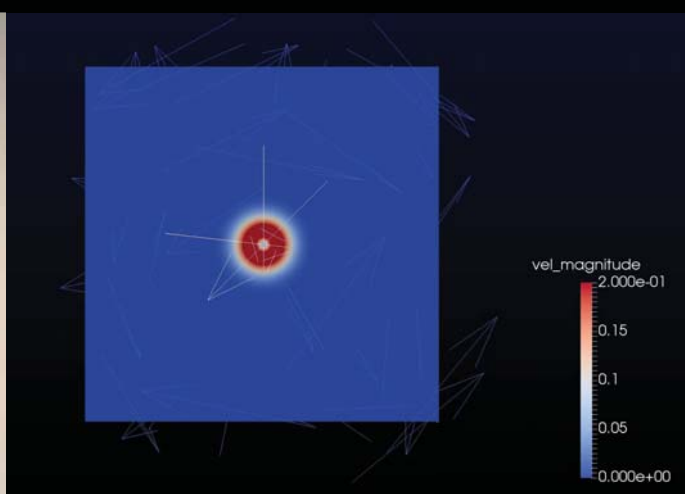
Both projects had a common objective to introduce in-situ visualisation techniques in the process of numerical simulation.

In situ visualization is a technique which allows scientists to explore the data while the numerical simulation is running. Furthermore, this approach allows to monitor and interact with the running simulation, allowing the adjustments of the simulation parameters on the fly so that the scientists can immediately observe the impact on the investigated phenomena.

This technique, by coupling visualization and simulation together, and over-coming the bottleneck of data transfer, can accelerate the computation and provide much better insight than traditional approaches.

The project 'In-Situ and Batch Visualization of Biogeochemical State of the Mediterranean Sea' has allowed to introduce the in-situ visualisation techniques in the 3D numerical model OGSTM-BFM used at OGS to study the nutrient and carbon cycles in the Mediterranean Sea and their sensitivity to climatic changes. The model computes bio-geochemical fluxes which transform organic and inorganic components.





Some pictures from the movie that won the best visualization award this year: A 3D rendering of the enstrophy in the fourier space (top). Cut of the magnitude and direction of the velocity field in the same system (down-right). Anurag Dogra, the student that won the prize (down-left).

During the two months at Cineca, the model has been instrumented for 3D in situ visualization, so the scientists are now provided with a tool which can be used to check and analyse the OGSTM–BFM model behaviour by consistently evaluating how the bio-geochemical processes are influenced by the nutrient and carbon cycles, specifically related to the three main boundary conditions: the Atlantic in-flow at Gibraltar Strait, the terrestrial inputs at rivers and the atmospheric deposition. The tool is also beneficial to control the correctness of the computations during the simulation runtime. Furthermore, the implementation has been designed in such a way that allows portability to other coupled modelling systems used at OGS for many different purposes.

The project "In Situ VIsualization of Navier-Stokes Tornado Effect" aimed at the numerical study of solutions of the Navier-Stokes equations for smooth initial data. These mathematical models have wide range of applications and, during the two months at Cineca, have been applied to Tornado simulations. Tornado is nothing but the rotating column of air which is in contact with grounds and cloud base. The evolution of a 3 dimensional vector field in real space has been simulated allowing to find the data to produced the velocity fields and enstrophy values. These values have been visualized with in situ techniques to better investigate the evolution of energy and the velocity fields of the tornado, using the ParaView tool and its feature Catalyst which acts as a medium of data transfer between simulation nodes and visualization nodes. The work produced by Anurag Dogra in this project has been documented in a video showing the in-situ visualisation of the tornado simulation.

The results achieved with SoHPC in Cineca were highly appreciated by the domain experts involved from OGS and University of Camerino who suggested respectively Petr and Anurag to continue the collaboration after the completion of the programme.

At the conclusion of projects, the Adjudication Panel, nominated by PRACE Management Board, assigned the SoHPC 2016 awards:

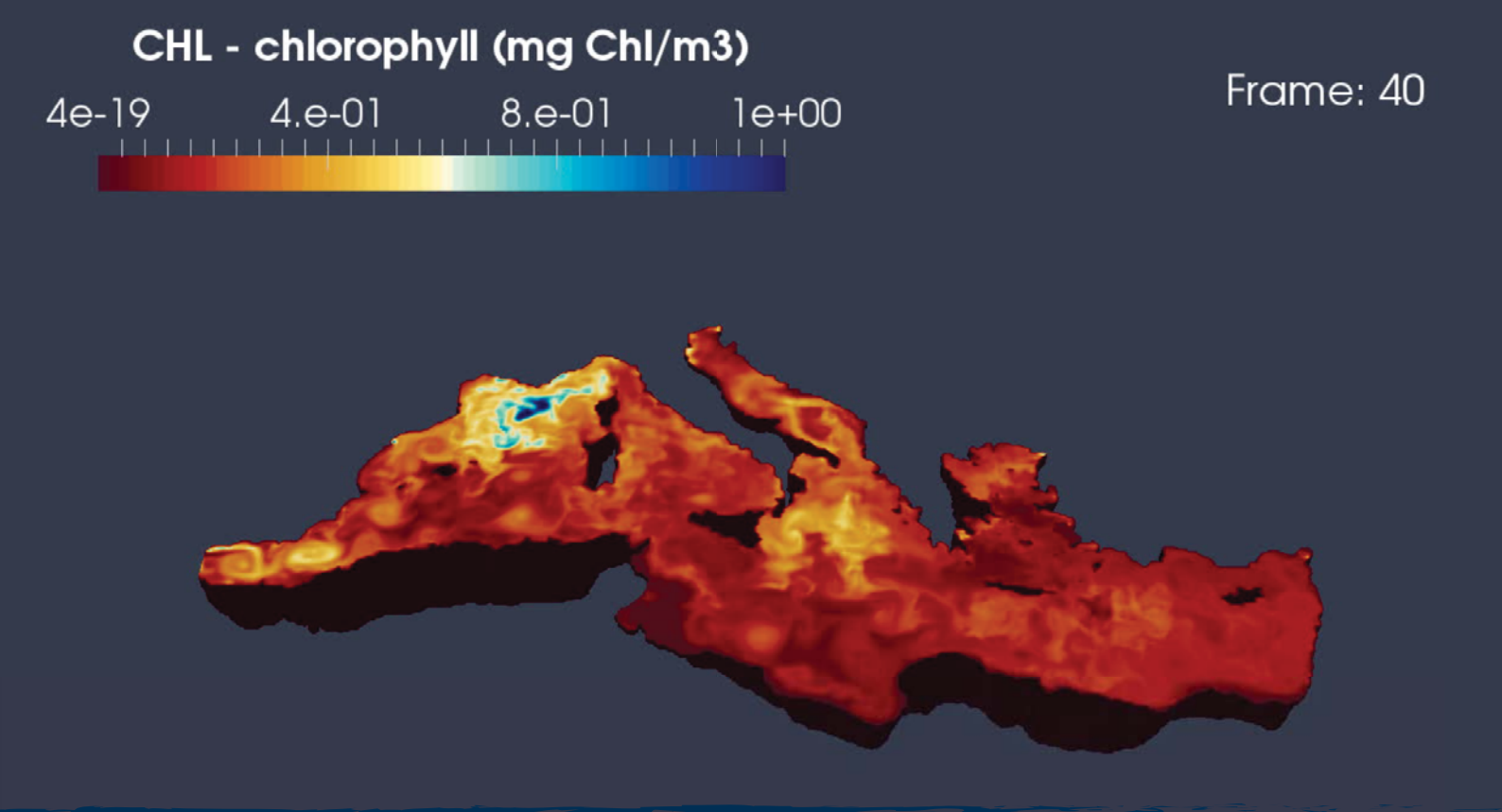
The Best Visualisation Award was assigned to Anurag Dogra. whith this motivation: "Anurag produced a highly impressive In Situ visualisation of tornado effects, in which he exhibited his dedication to quality. His visualisation very nicely explained the complexity and journey of working in High Performance Computing. He exhibited great understanding of the underlying physics and produced an excellent report. He received very positive feedback from his mentor and fellow participants. The high quality work illustrates his motivation and dedication to the programme. Anurag was excellent team player that contributed strongly to the Summer of HPC".

Marta Čudova, a student from Brno University of Technology in Check Republic, who spent the summer at the research center EPCC in Edinburgh received the HPC Ambassador Award for her "strong motivation and commitment for promoting HPC throughout the SoHPC programme. She bridged CFD and image reconstruction codes using parallel Python. Moreover, she successfully communicated the importance and objectives of her project through her blog posts and video and promoted them through social media. The quality of her blogging was excellent and reached a wide audience. Marta fully embodied the outreach spirit of the SoHPC programme".

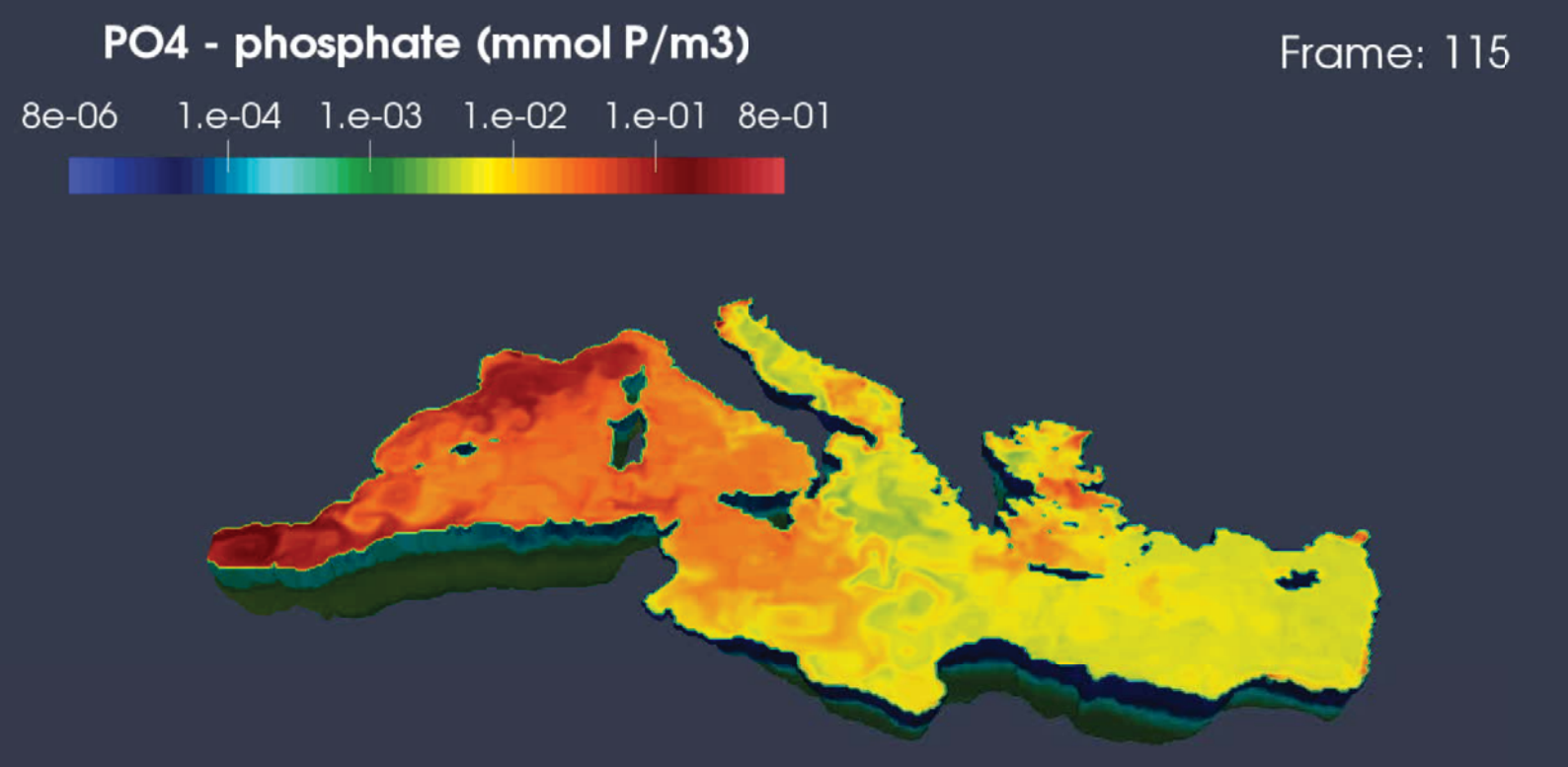
For SoHPC 2016 the Awards ceremony was organised in Cineca on December 1st.

SoHPC represents a great occasion not only to fascinate students in computational projects and outreach activities, generating new interests in HPC and exchange of knowledge between young researchers, but also a big instrument to communicate HPC and to strengthen cooperation at the European level.

Giovanni Erbacci
Cineca



3d maps of chlorophyll (top) and phosphate (bottom) concentration fields in the Mediterranean Sea. Areas with an intense biological activity, characterized by high chlorophyll concentration levels, are driven by vertical mixing of nutrients (phosphate shown).



Big Data

In a large number of domains, the exponential growth of data generated and collected enables processes of data driven innovation which have a potential to contribute to productivity, well-being, inclusiveness and development. For many of the steps in the value creation process along the data value cycle, researchers and organizations have to involve third parties, as they lack experience and/or technological resources. This gives rise to a global data ecosystem in which data and analytic services are traded and used across sectors and national borders. During 2016 we consolidated our position in this global data ecosystem as an infrastructure provider offering data management and analysis tools and critical computing resources (storage and cloud computing resources) and we increased our visibility by participating to various big data communities at regional, national and international levels.

The newly implemented SCAI data centric model has been successfully exploited by all scientific communities, with a new emerging one: the Bioinformatics community. In 2016 Cineca, became partner of the Italian node of Elixir, the European infrastructure for Bioinformatics, with a collaborative pilot project that provides access to the digital infrastructure for HPC and data processing and management to the national users community. Bioinformatics now ranks as the fourth domain by storage consumption after the HPC traditional domains of Earth and Climate, Astrophysics and Computational Fluid Dynamics. Data are mainly coming from Next Generation Sequencing and make extensive use of the analysis pipelines that are already integrated in the platform. A genome repository is being developed in collaboration with Telethon to host the Italian genome sequences, beginning with those generated by the research on rare diseases.

Beside providing training programs and technical support on the infrastructure, middleware services and advanced data analytics software, in 2016 we were involved in individual big data projects (Reggia di Caserta), open innovation projects (TEXA) and joint experimentations (ISTAT), dealing with social media, web pages and sensor generated big data.

In the first case, data from social media were collected and analyzed to provide the Caserta Royal Palace with a real time reputation monitoring system, that is also interactive on historical data and past events. The system tracks the topics being discussed and the sentiments being expressed and can be used to assess the impact of events and communication strategies.

In the second case, the PRESERVE project, which is funded within the Fortissimo EU project, sensor data from TEXA on-board diagnostic tools are analyzed in order to identify the driving habits on one hand, and patterns of operating parameters that are predictive of failures and damages on the other hand. The aim is to map the vehicle "DNA" in normal conditions and thus to be able to detect deviations towards the "disease" status. If successful, this would become a data-driven service that TEXA could sell to vehicle manufacturers.

Finally a joint experimentation with ISTAT has started in order to assess Internet as a data source for the production of Official Statistics. This collaboration aims at identifying the data sources and the processes that can be used to provide accurate and reliable statistics. The National Statistical Office defines the phenomena to be monitored, provides the "ground truth" (data from surveys), and evaluates the results. Other stakeholders might be identified depending on the phenomenon under study.

In 2016 the research activity focused on the integration of web scraping, text mining and machine learning techniques in order to obtain the estimates currently produced by the "Survey on ICT usage and e-Commerce in Enterprises". The web scraping procedures, covering 10289 web sites, each of them contributing around 1000 pages, and more than 200 million textual records, have been optimized on PICO.

The aim in all of these projects is to develop new analytics tools and services leveraging on HPC and Storage infrastructures in such a way that they will be reusable also in other contexts and also to make the HPC environment more attractive for the non-traditional-HPC-users.

Roberta Turra
Cineca

ISTAT

Since 2013 Cineca started a collaboration with ISTAT to investigate the use of web scraping techniques, associated with text mining algorithms, in order to replace traditional tools of data collection and estimation, and/or to combine them into an integrated strategy. This collaboration took place considering that the amount of information accessible through Internet is an enormous resource, useful to describe many aspects of the present society. The possibility to extract this information has several benefits, including a "constant measurement" of a given phenomenon, or the replacement (total or most probably partial) of surveys able to measure it. Indeed such a process presents new challenges, due to that fact that the traditional methods have to deal with an unstructured information, often huge and sparse. But this challenge is in line with the new approach defined "Internet as Data source" (IaD), that currently many National Statistical Institutions are studying to provide policy makers with data to propose and monitor policies. The first results of the collaboration between ISTAT and Cineca is represented by a joint article named "Web scraping and web mining: new tools for Official Statistics", presented in the 47 Scientific Meeting of the Italian Statistical Society. In such study, a sample of 8,600 enterprises' websites were "scraped" and the acquired texts processed in order to attempt the collection of the same information gathered via the standard questionnaire related to the ISTAT sampling "Survey on ICT Usage and e-Commerce in Enterprises". The preliminary results were quite encouraging, stating an almost satisfactory predictive capability of the fitted models. Such experience was repeated in the following years, by considering new methods to collect the information from internet and most advanced paradigms to extract automatically the proper characteristics for each enterprise. It has to be noted that, despite the objects of this analysis (a small sample of the Italian enterprises) are limited, the quantity of information that can be derived for them from the web is huge and changes rapidly over time. This is in line with the Gartner's definition of Big Data, that considers "high-volume, high-velocity and/or high-variety information assets that demand cost-effective, innovative forms of information processing". Within this experience, Cineca was able to develop its own methods able to transform unstructured information in structured; moreover, the possibility to use the supercomputers, resulted in significantly reducing the needed computational time, in respect to what can be obtained by normal PCs. From the point of view of ISTAT, instead, the obtained results were able to open new fields of research; between these, one is related to a more extensive application of the approach in a "Census like manner" (for instance, by considering all the enterprises in Italy instead of a sample of that). But, more important, this new methodological framework requests from ISTAT the definition of new statistical strategies that should be used to evaluate the reasonability and the quality of the results. In this last year the results of a new study was presented during the seventh international Conference on Agricultural Statistics: "ISTAT Farm Register: Data Collection by Using Web Scraping for Agritourism Farms". The idea of this study was the possibility to not substitute the original source of information by means of internet, but to extract from it additional information. In particular, the research investigated the possibility to identify specific characteristics of all the Agritourism Farms in Italy referring to one of the main hub websites for travelling (Tripadvisor), or by using directly the web site of each farm. Also in this case the results were quite encouraging, showing the possibility to update also a series of information that were specified only when the farms registered themselves in the administrative archives. In this last year ISTAT and Cineca decided to further formalize the collaboration by signing a research agreement and by defining new research objectives and a more appropriate use of computing facilities. Among the new objectives, the possibility to classify satellite images, in order to identify the characteristics of the land cover.

Giulio Barcaroli
ISTAT

Marco Scarnò
Cineca

A new digital ecosystem for Caserta Royal Palace

Aiming to promote its cultural heritage, the Caserta Royal Palace has become a "playground" for experimenting innovative technologies using 3D reconstruction, big data and sentiment analysis. Beginning with the modeling of the "Terrae Motus" exhibition, the project aims to create a "sentiment room" where it will be possible to browse digital contents, and sentiments, about the Royal Palace.

To project an exhibition, or setting up a new path in galleries, usually involves museology, museography and some experienced and outdated techniques. By using the Blend4Web framework and a collection database, the exhibition can be built in an innovative way, changing also the way in which museums communicate heritage and document exhibitions.

Caserta Royal Palace has set up the temporary exhibition of "Terrae Motus", the Lucio Amelio contemporary art collection that was gifted by many of the most important artists at the end of last Century, after the terrible earthquake in Naples area. The exhibition take place in the Royal Palace area that was previously occupied by Aereonautica Militare.

Using Blend4Web, an open source Software Development Kit for the creation of 3D web pages, we have built the rooms model, and we have placed the artwork creating the replica of the exhibition, that can be viewed also when it will end. Even more, the 3D reconstruction of the rooms is an operative tool for setting up the next exhibitions, giving to curators an effective and powerful aid for their work.

Caserta Royal Palace has initiated a challenging collaboration with Cineca, aiming to exploit the most advanced technology at heritage service. The starting points of this experiment were two: the setup of the temporary exhibition of the Terrae Motus Collection, and a sentiment analysis that evolves in the Royal Palace social networks streams.

Terrae Motus Blend4Web Virtual Exhibitor

The reconstruction of existing models requires a great deal of information in order to assure the greatest possible degree of accurate details, thus lending more realism to the virtual reconstruction. Our first step was the definition of the 3d museological space, for which we chose the Caserta Royal Palace's rooms dedicated to the Terrae Motus exposition. This reconstruction was driven by the existing CAD files of the building's two floor plans and both sections for the volume of each room. The CAD files were based on the relief made by Rome's La Sapienza University and the government ministry responsible for stewardship of the environment and historical buildings. That project team was supervised by Cesare Cundari, in 2005[1]. After the definition of the 3D space through photogrammetry, every architectural detail had to be textured in order to achieve the level of realism that allows users to recognize a particular room of the exposition. The virtual exhibitor is a web application allowing interested visitors to experience the exhibit in an interactive videogame-like 3d visualization, directly within any web-browser, with no need to install additional plugins. This experience is possible with any device, including the pc, the tablet and the smartphone. The technology behind the Exhibitor is based on Blend4Web[2] : an effective tool that allows exportation of Blender contents to web pages, and provides state-of-the-art WebGL rendering capabilities, as well as sound support, animation, and scriptable user interaction.

In order to support less powerful devices such as entry level smartphones, Blend4Web offers a set of quality-profile setups, and automatically chooses the one most appropriate for a given device.

The second phase of our work was the definition of which paintings, statues or special installations to be put inside the 3D space.

The anticipated use of the dynamic 3D model built in this project is as an operative aid in planning exhibitions. Once the gallery's realistic 3D model and the database of its potential contents have been created, the curator can arrange the works in the space or on the wall; room dividers may also be set up quickly in the 3D model in order to convey the atmosphere of a temporary exhibition. Curators may arrange, rearrange and perfect the exhibition however they like.

Up to now, the documentation of temporary exhibitions has been primarily through the publication of an exhibition catalogue. Building 3D models of temporary exhibitions provides a more performative documentation of such events, while also furnishing educational material for museum studies and researchers. The most immediate advantage of this 3D model, however, is to better communicate the exhibition on the web, encouraging and enhancing visits to the actual museum.

One of the exhibition room (Racchetta Room) with paintings in one of the possible arrangements. Simulation of the Virtual exhibition, with the required information given during the real time navigation.

Sentiment Analysis

Tourism has become more and more an emotional experience rather than a simple trip. An understanding of the ways in which tourists experience the places and people they visit is fundamental to the study of the conception of tourism. It is not surprising that attention has long been paid in tourism literature to particular perspectives on the tourist experience, including the role of new media in cultivating the image and perception of the Caserta Royal Palace. Facebook, Twitter, TripAdvisor and more generally all the social networks are the new online word of mouth. The ability to decipher emotions, opinions and judgments that lie behind a post or a tweet is the real value added of these data sources. Since large numbers of posts or tweets do not always indicate positive reception, the main goal of our Sentiment Analysis reading this exhibition has been to determine whether the expressed opinion in these texts is positive, negative or neutral. We analyzed 7,500 Facebook users who, from 2012 to August 2016, posted or commented on more than 17,000 instances of content; more than 10,500 Twitter users from March to August of this year who tweeted almost 25,000 times; and nearly 3000 Tripadvisor reviews for a total of 45,000 interactions. 227,000 words from these communications have been analyzed and classified.

The main finding is that The Royal Palace of Caserta is objectively beautiful in the perception of its visitors.

Tourists (potential or actual) register an overall positive sentiment of 71/100. Facebook reaches a value of 83/100 while Twitter is more sensitive to facts and events that influence negatively on the indicator (59/100).

The data attest to positive visitor reception regarding the Palace's activities and events (88/100), hospitality (76/100), location (64/100) and accessibility (60/100); visitors express need for improvements in catering (48/100) and prices (37/100).

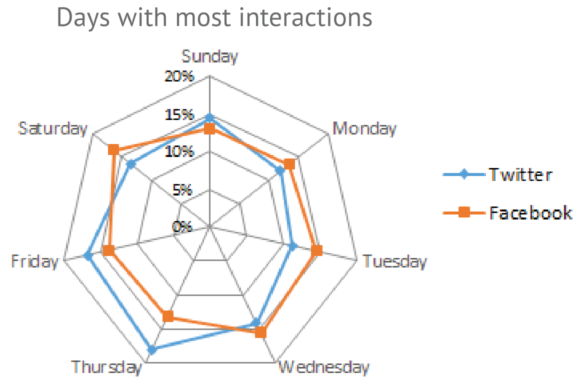
In this paper we have been able to present only a few instances of our integrative model, but the big picture that is at the basis of the agreement between the Caserta Royal Palace and Cineca is another matter. The 3D model of the Terrae Motus Exhibition is only the beginning of the 3D modeling of the whole Palace, which will be integrated with: infrastructural data, such as electricity cables, water pipes and services; surveillance camera data; details about the statues, paintings and other artworks shown in the Palace, including descriptive metadata, in a complex BIM model, enriched with heritage information. This 3D model can be installed in a sort of "sentiment room," where screens may display real time images of activities in the building, including the overall sentiments that people convey regarding the Caserta Royal Palace through live tweets, "likes" and comments on Facebook, pictures on Instagram, and opinions on Tripadvisor.

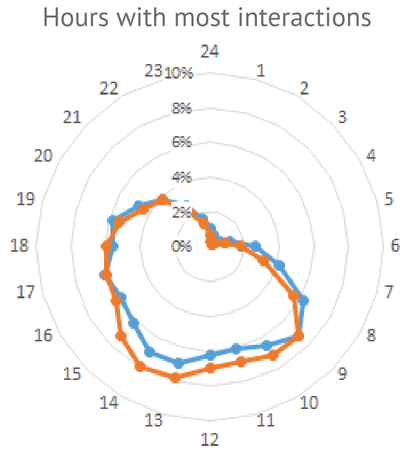
Mauro Felicori
Caserta Royal Palace Director

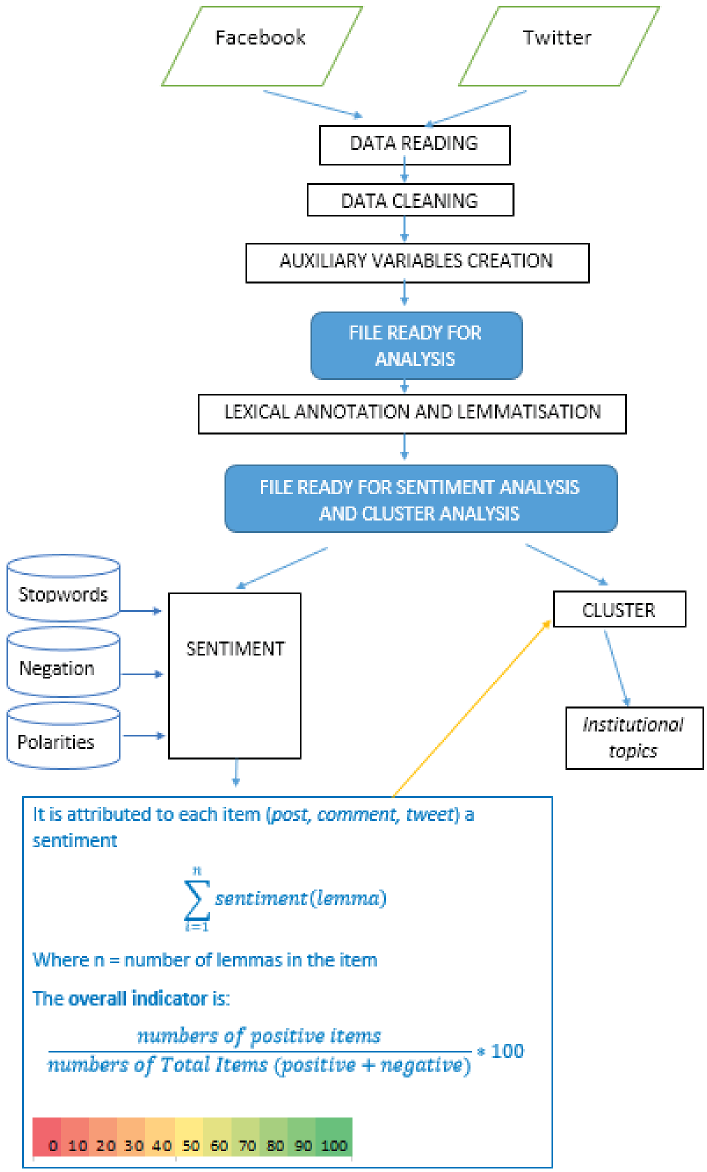
Antonella Guidazzoli
Donatella Sforzini
Cineca

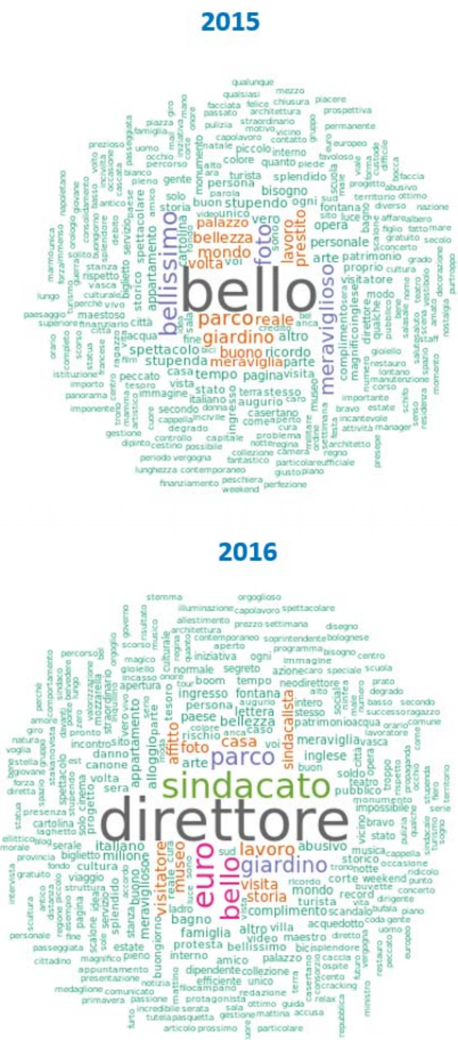
References

[1] C. Cudani (ed.), "Il Palazzo Reale di Caserta", Roma, Edizioni Kappa, 2005
[2] https://www.blend4web.com/en/









Caserta Royal Palace sentiment analysis: statistics on interaction (top), workflow (left) and tag cloud (right).

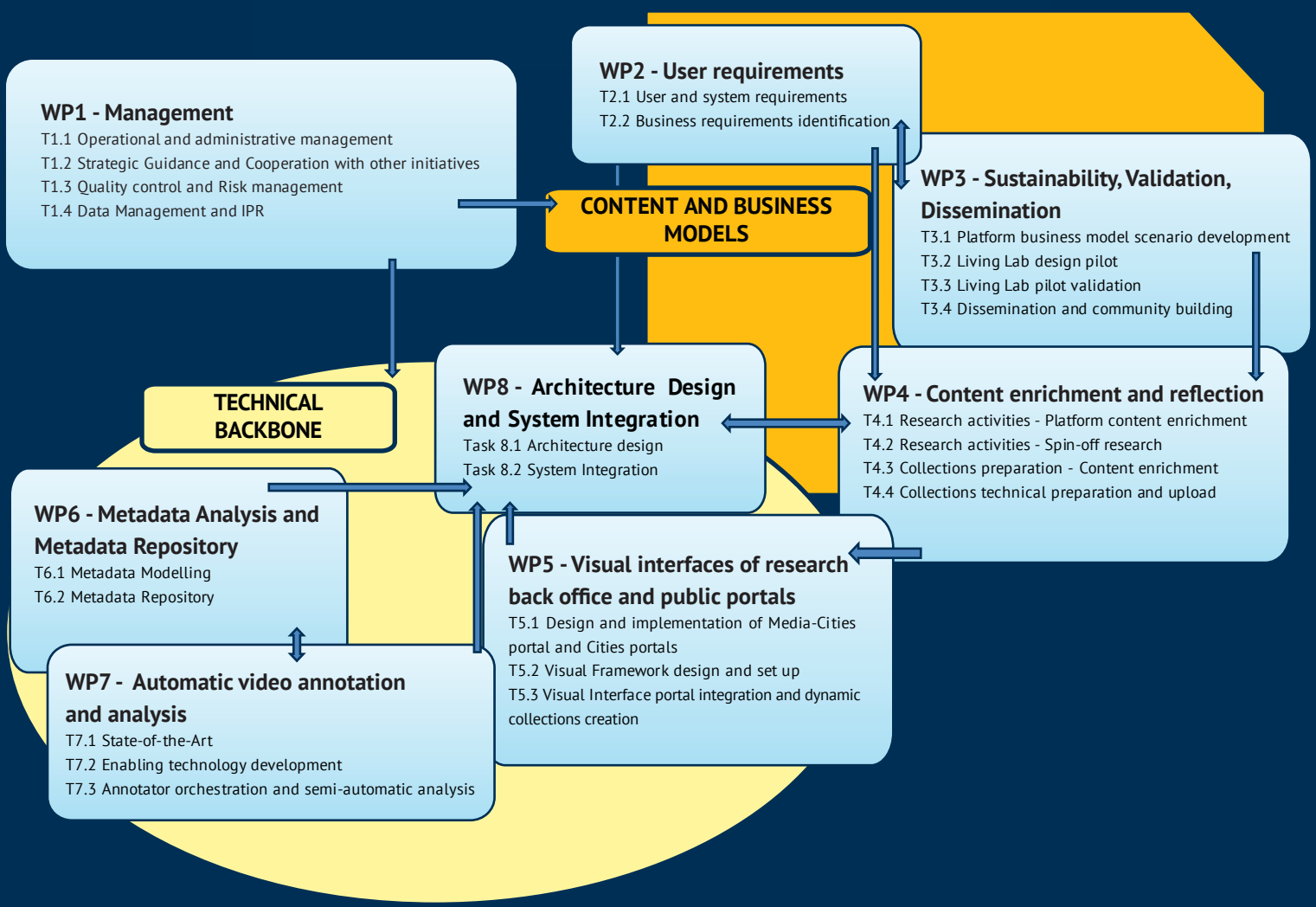
Data In Social Sciences And Humanities: I-Media-Cities

Big data in Social Sciences and Humanities (SSH) has tremendous potential for social and economic impacts and it is strategic for the transmission of European cultural heritage, history and identity, and for enhancing creativity.
These data do not only deal with large and networked cultural datasets, but also call for new study and interpretation methods in the SSH.
In this context Cineca recently presented "I-Media-Cities", a H2020 project funded under the Reflective-6-2015 call.
I-Media-Cities is an ambitious and innovative research project led 9 European cultural institutions (film archives from 8 countries), 5 research institutions, 2 technological providers (Cineca and Fraunhofer) and a specialist of digital business models, to share, provide access to, and use their digital content, turning it into the lever of novel approaches to multidisciplinary research, to business innovation and to the overall accessibility of the European cultural heritage.
As an experimental innovation action, the project focuses on the digital content that revolves around cities in European history and identity. A huge quantity of fictional and non-fictional AV works in institution collections describes cities in all aspects, including physical transformation and social dynamics. Such material could prove of enormous value to scholars in different fields of study.
I-Media-Cities plans integration and technical development work to generate two types of e-environments to be used by researchers and innovators. This is meant to integrate new digital assets and construct an open and co-creative and competitive European ecosystem involving citizens in the annotation of the contents, applying the paradigm of open science in reflecting on european history and identity.
This will allow new approaches to research in social sciences and unleash creativity, in new forms of delivery and consumption of that contents which the creative industry would be able to propose for instance in tourism or in the cultural economy.
At the end of the project, we will deliver a digital content access ecosystem, made available to a growing community of researchers, to push the boundaries of what we can learn, through AV material on cities, on European history and identity. The legacy of I-Media-Cities will be a new model for research on digital sources (applicable also to other subject areas), plus appropriate exploitation plans to consolidate and expand the platform into the European reference initiative on AV digital content.
On the side of research methodologies, the project will become a reference for new research-driven approaches to collection management, digitization and access from large organizations, while currently moving image material has no real impact on research as it is largely unavailable.
Technological solutions implemented in I-Media-Cities will make completely new approaches to research on moving images possible that are now unavailable to scholars. For example, scene detection and document fragmentation of clips will provide unprecedented levels of granularity for research and visualization purposes. Further AV content analytical tools will be offered to the researchers.
Also, annotations and tagging from scholars and researchers will become integral part of the metadata processed by the system. The Data and Metadata Central Repository will store and organise all the information gathered from cultural institutions, researchers, citizens and extracted by automatic analysis tools in a complex and innovative way.
Finally, new ways to display and visualize contents, will provide unprecedented possibilities to analyse moving image content enabling totally new paths to analyse, study and explore large moving image collections.
These new models and paths will not be limited to the subject matter chosen by the project, but may bear impact on the whole field of social sciences through the lenses of audiovisual material or digital collections in general.

I-Media-Cities web site project: https://imediacities.eu/

Gabriella Scipione
Antonella Guidazzoli
Cineca

i media cities



Performance Measurement for Strategy Development

In 2016 SCAI started a project to construct a performance measurement system (PMS) for supporting its strategic development and assessing its project and activities on a continuous basis. The project is carried out in collaboration with Politecnico di Milano, Department of Management Economics and Industrial Engineering.
The project is indeed an innovation for SCAI, and, in general, it is also an innovation at the methodological level. SCAI has in fact decided to invest in internal human resources and to create a team who follow the project under the supervision of Politecnico di Milano. Furthermore the Head of SCAI actively participate in the project development. Consequently, an action learning approach is entailed, where Politecnico di Milano and SCAI cooperate, alternating sections of informal learning and field action. This method implicates a longer duration of the design phase, but favor the increase of capability of personal and a better personalization of the PMS. A second methodological challenge is linked to heterogeneity of SCAI. SCAI is characterized by great variety of activities; they provide services and resources for HCP on a routine basis, but they carry out research projects of various nature. The expected performances for these areas are different as well as the strategic reflection needed to stay competitive. In face of this challenge the project adopts a modular approach, where the identification of responsibility centers will be crucial.

The project consists of three phases:

1. Strategy mapping; in this phase, the research team, analyse the current SCAI portfolio and map the strategic development highlighting: project and routine activities; critical success factors for each area analyzing the external and internal environment; entail the future positioning of SCAI, this phase started in December 2016.
2. Identification of responsibility centers; the second phase is more internally oriented and aims at identifying the resources devoted to each project/activity area. This initial analysis allows to assess the coherence between the future strategic positioning and available resources.
3. Construction of the performance measurement system. This last phase is devoted to the definition of performance indicators to measure for SCAI at the overall level, for each responsibility centers and for project and activities.

The output of the project will be a PMS for SCAI that can be used for planning, measuring and reporting the results of action to various stakeholders (Figure below).

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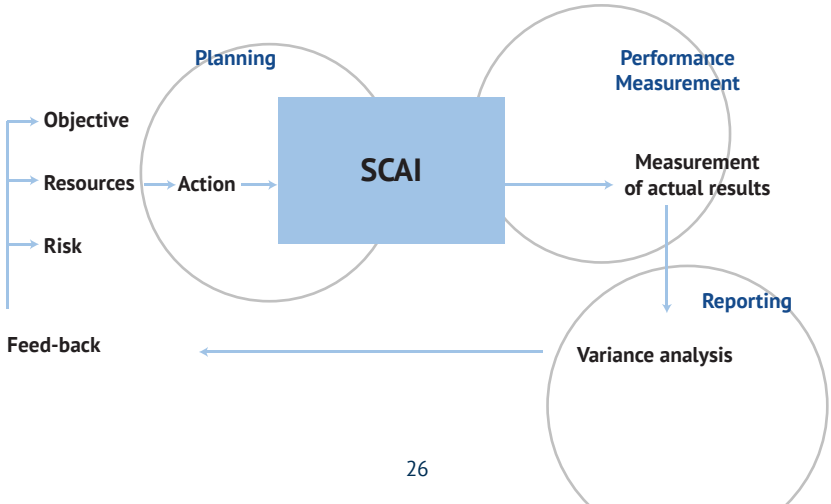


2016 SCAI at a glance

Being the italian HPC reference and staying competitive in the world

12
in the top500 ranking

2286
active users

1140
projects supported

860M
core hours consumed

- Directly involved in:

  - 31 EU research projects
  - 40 research agreements with relevant national institutions
  - 12 applied research projects with industrial partners

To support Italian researchers to face global scientific challenges

- Computational Chemistry
- Computational Fluid Dynamics
- Condensed Matter Physics
- Computational Engineering
- Astrophysics and Plasma Physics
- Earth and Climate Science
- Life Science

The backbone

- Cultural heritage
- Bioinformatics
- Industry4.0

Big data and Machine Learning

2016 HPC in numbers: usage & users of our infrastructure

Our access policy and resource management

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

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

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

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

Our users

During the year 2016, we acquired about 400 new users for our HPC systems, the total number increasing from 1.877 to 2.287.

The registered users in our DB exceed 3.200, 2.287 of them are actively accessing the HPC resources, some accounts being expired (no access for more than one year) and some others never finalizing their enrolment. The large increment (last year only 200 new users enrolled in the period) is mostly due to the inclusion of a new community (EUROfusion) that started mid 2016 using the MARCONI cluster.

Not surprisingly, the great part of our users are males and Italian (80% and 75% respectively - see Figure 1). As far as the researcher gender is concerned, the figure is substantially unchanged with respect to last year, while the number of international researchers is increasing (from 22% to 25%), thanks to the presence of the truly international community of EUROfusion.

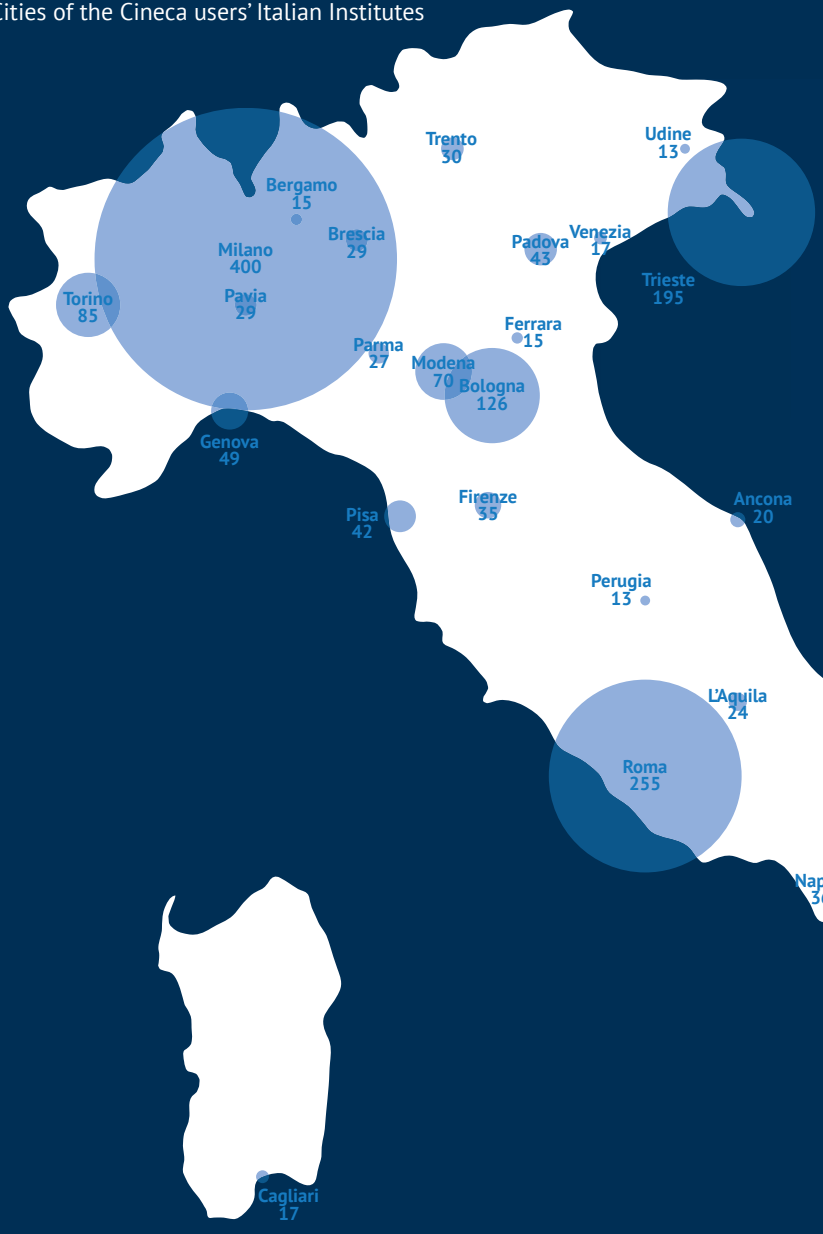
Among the more popular foreign nationalities: Germany and France, followed by Spain and United Kingdom, but also China and India are well represented.

The great majority of our active users belongs to Academic or public and no-profit Institutions, the private users representing a really small part.

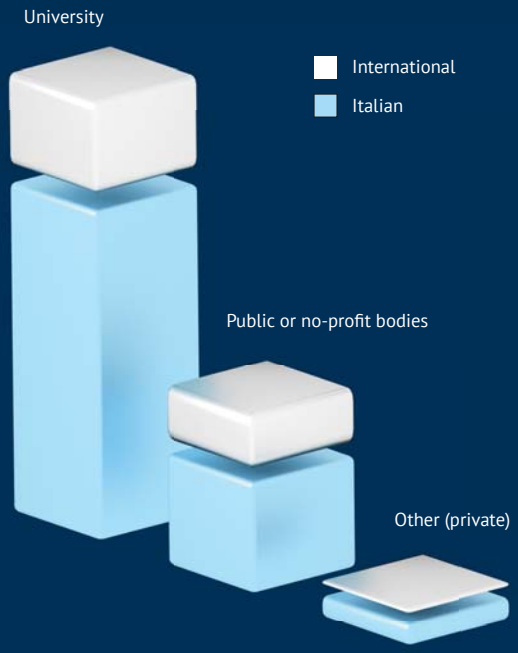
The large Italian cities, aggregating several Research Institutions, are well represented: about 500 users come from the Milan area, 255 from Rome, 195 from Trieste (University, Sissa, ICTP, OGS), about 200 from the Bologna and Modena area 85 from Turin, nearly 40 from Padova, Firenze, Genova, Pisa and Naples.

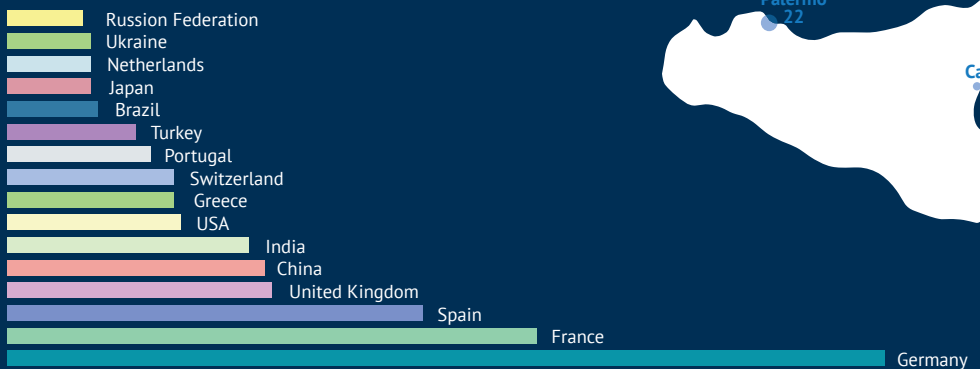
As one might expect, the great majority of the users are scientists: Chemistry and Condensed Matter Physics still remains among the more traditional and populated disciplines (see figure next page). The first research field is however Particle Physics, for the first time this year (22%), thanks to important collaborations with INFN (National Institute for Nuclear Physics).

Cities of the Cineca users' Italian Institutes

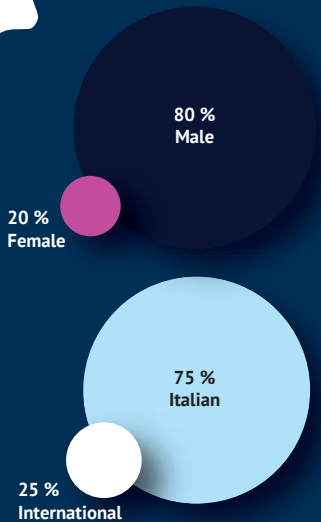


Classification of Cineca users institutes





Nationalities of Cineca users



Number of Cineca users divided by gender and nationality

Allocation programmes

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

During 2016, a total of 1,6 billion core-hours has been distributed on the old Tier 0 machine (Fermi – in production up to June 2016), the new Tier 0 cluster (Marconi – in production since July 2016) and the Tier 1 cluster (Galileo).

The PRACE projects (referring to the European HPC infrastructure) was awarded with the 71% of the resources and ISCRA projects (targeted to Italian researchers) took the great part of the remaining availability (29%).

In the same period, a total of 658 Million core-hours were used on FERMI (an average of 94 Million per month for the six months' production in 2016), 80 Million core-h on Marconi and 54 Million on Galileo. In the figure in the following page the monthly distribution over the three clusters is presented as an average monthly value, distributed into the main allocation categories.

The LISA regional Programme has been resumed during 2016, but the resources consumed on the HPC clusters are too small to be visible.

How computational resources have been used

During 2016, a very important change occurred in the equipment organisation of our computing room. A very large system, Fermi, with a capacity of 1.5 billion core-hours per year was substituted by Marconi that in its first phase, is able to deliver only 1/3 of such capacity. Only with the second phase, in place from January 2017, the total capacity of Marconi will supersede the former one, with a value of more than 2.5 billion core-h per year.

a comparable value (Galileo (in its research partition) is a 6784 cores system with a total capacity of 60 million core-hours per year.

The three available systems (Fermi, Marconi and Galileo) have been fully exploited during 2016, taking into consideration the six months' production of Fermi (January to June) and Marconi (July to December). Fermi reports a global use percentage greater than 94%, Galileo 98% and Marconi (considering its new availability) 62%.

The User Support

Cineca puts a strong effort in the support of the users. This has always been for us a crucial task for assuring an effective service for the research community. A number of professionals, trained in technical and scientific topics are working within a schedule to ensure the Help Desk presence during working hours. The support is operated through a Trouble Ticketing system available via email (superc@cineca.it).

The Help Desk service is governed by a ISO9001:2008 procedure, for the quality management, defining the process with KPI (Key Performance Indicators) and related target values, such as all tickets must be taken into consideration within a working day.

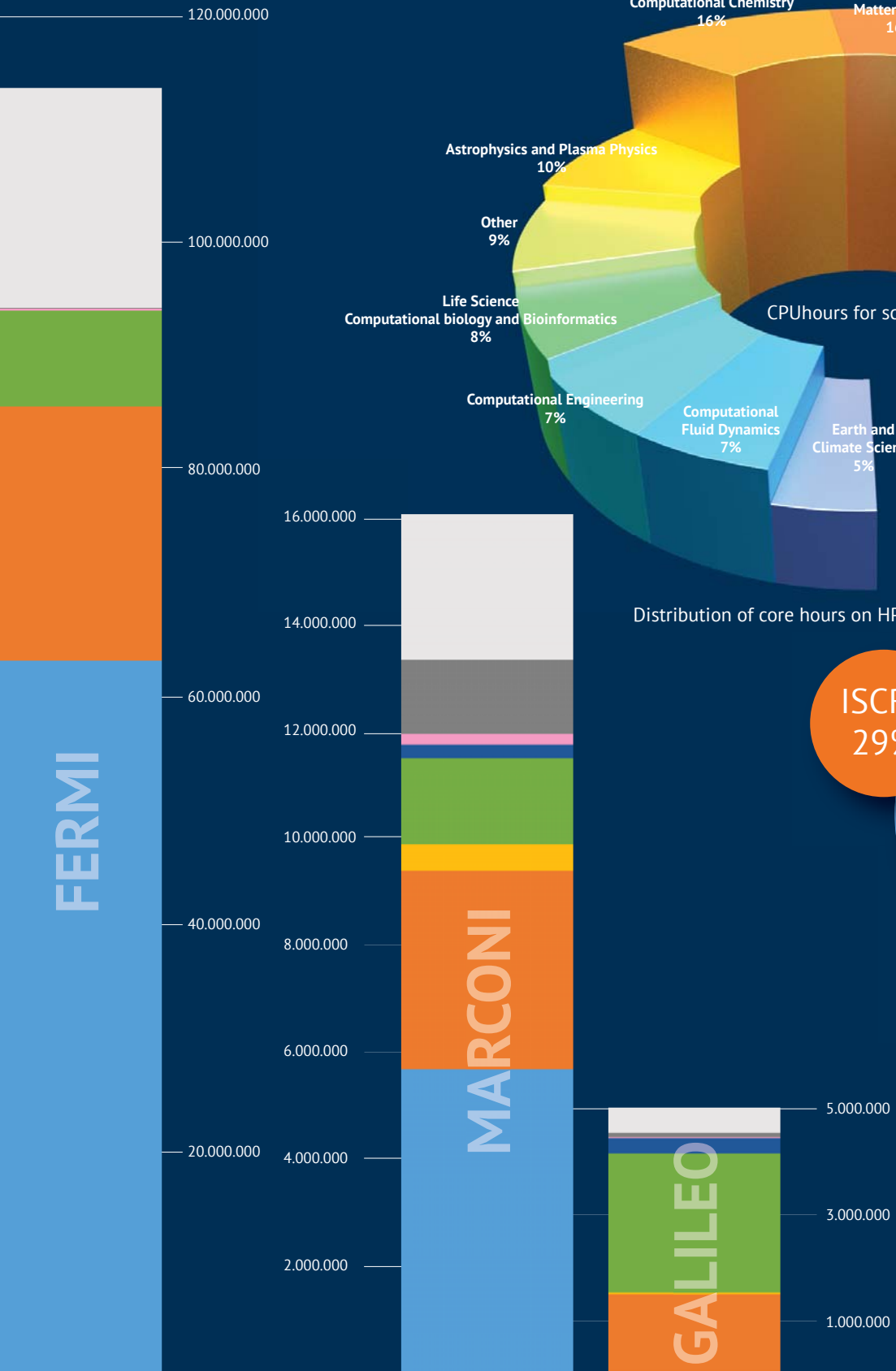
During 2016 a total of 3350 contacts were received, reporting problems (34%), service requests (28%) and information requests (38%). The average time for taking the request into account was less than one hour, with a descending trend over time.

One of the tasks of the Help Desk team is the installation of applications, tools and libraries on the HPC systems. This is done within the "module" framework, assuring the simple and easy access to common tools. All the software applications available are described in our web site (www.hpc.cineca.it/content/software) and a comprehensive documentation on their use is available on the HPC platforms.

Tools for developers are available (compilers, libraries, debuggers, profilers) as well as scientific applications spanning different scientific fields: Chemistry, Physics, Life Science, Bioinformatics, Engineering, Astrophysics, etc.

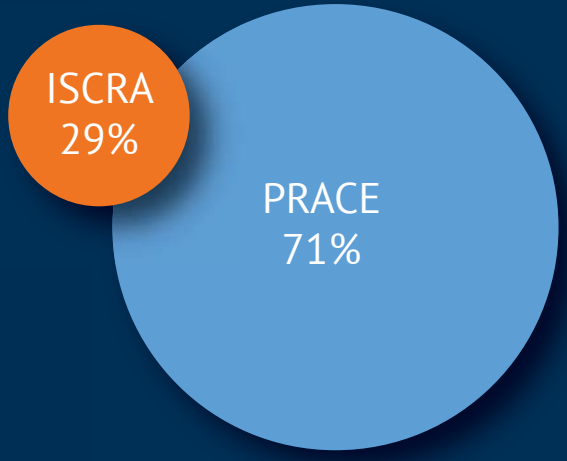
On each system the best suited applications are pre-installed, for example on Marconi the user can find only applications with a very good scaling behaviour, while Galileo hosts more general applications.

Core Hours production on Fermi (Tier 0), Marconi (new Tier 0) and Galileo (Tier 1) in 2016, on a monthly base.



CPUhours for scientific area of Marconi and Galileo, on a monthly base.

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



- PRACE
- ISCRA
- AGREEMENT
- LISA
- PROJECT EU
- CONTRACTS
- INTERNAL
- IDLE

Training

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

During 2016 we reached quite impressive numbers: 15 courses, distributed in 32 different editions, held in the three sites of the consortium, Bologna, Milan and Rome; 4 schools in 5 editions and 1 workshop. 50 people in the SCAI Department contributed as teachers, for a total of 150 days of lectures and highly specialized training. In total, over 760 Italian and European researchers had benefited of our training program. Students appreciate these courses and the surveys show high satisfaction levels, reporting an average rating of 8.5/10.

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

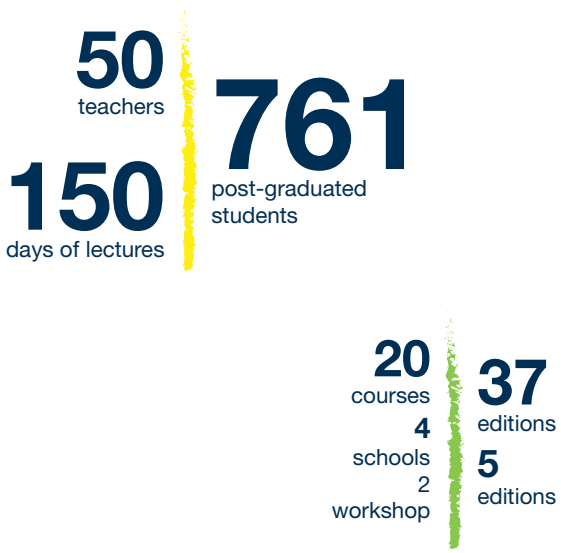
Besides traditional lectures, many other initiatives attracted very young promising scientists to Cineca, to spend short or extended visits under the mentoring action of our experts, who help them to maximize the output of their research or enhance their expertise in HPC techniques.

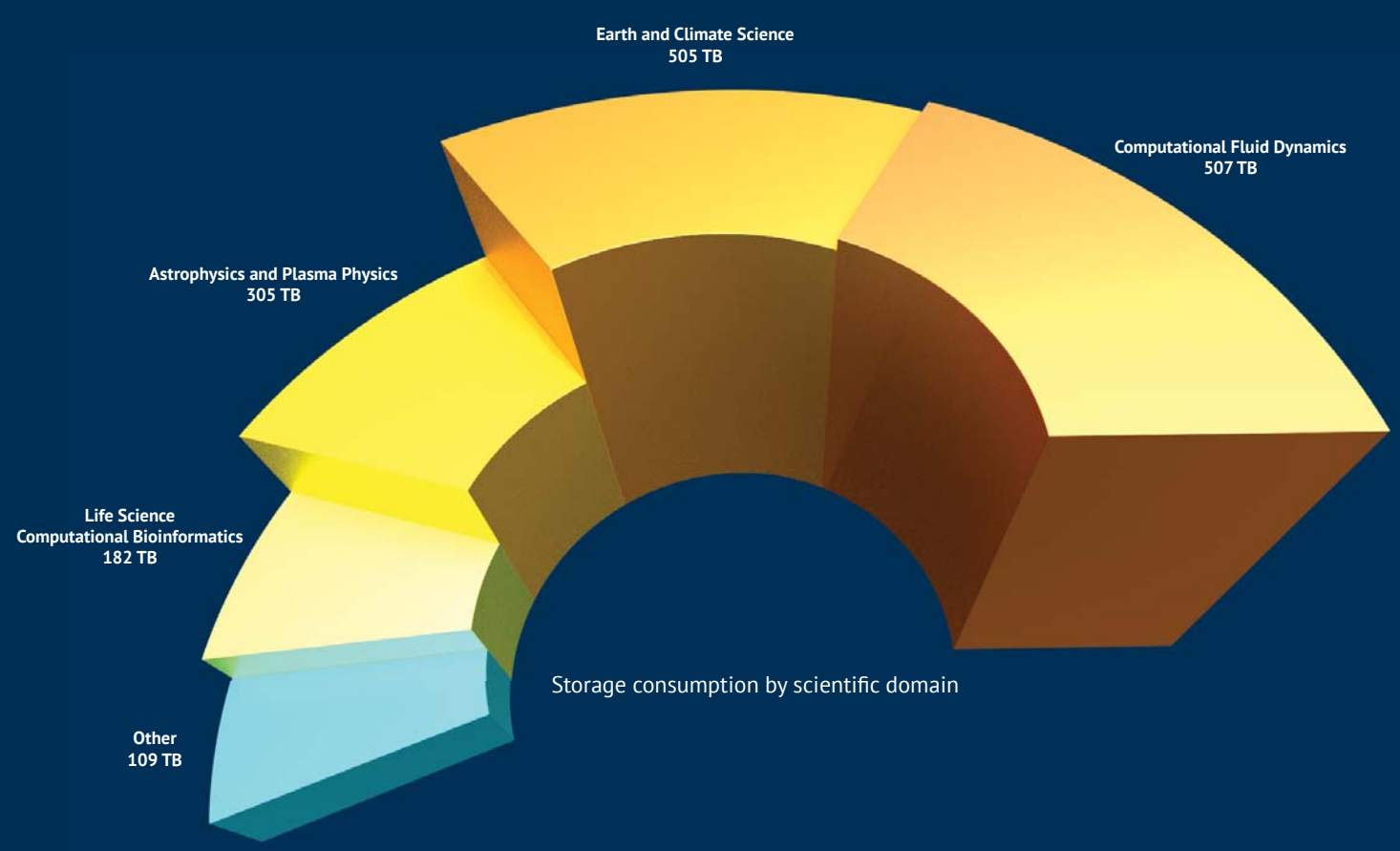
Also this year we took part in Summer of HPC (SoHPC), a PRACE initiative offering young University students from all over Europe the chance to do internships at major computer centers in Europe in the months of July and August. In the summer of 2016 we hosted two students. Their experience is described in detail in a dedicated section of this report.

Elda Rossi
Claudia Truini
Cineca

Numbers:
20 Courses (37 editions) (10 Courses PATC)
including:
4 schools (5 editions)
2 workshop

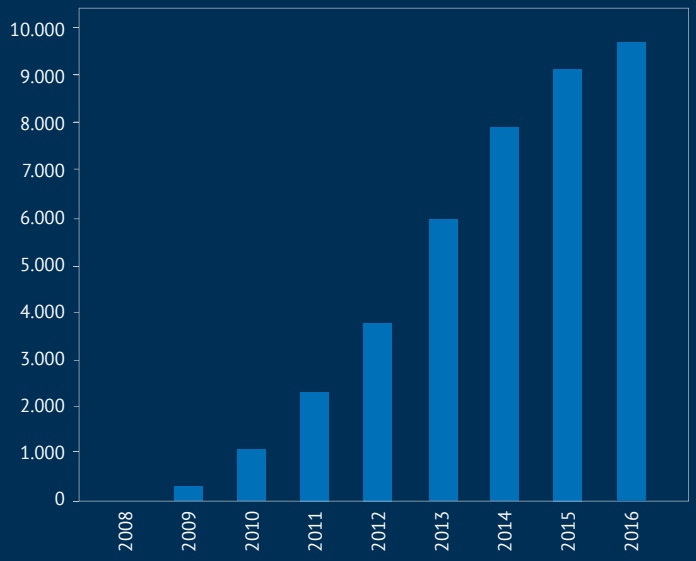
761 students





Scientific publications

Citations

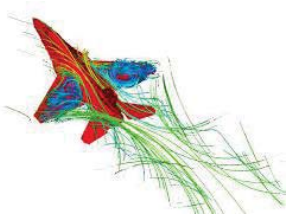


Number of scientific publications produced by Italian scientists acknowledging the resources granted by Cineca and number of citations. Information extracted from the reference database "Web of Science", analyzing the publications using HPC technologies in all the science and engineering fields. On a seven years time-span, 2008-2015, we got 2.465 publications mentioning Cineca as funding source.

97% of all publications have at least one author from an Italian organization. Among the authors coming from foreign countries, the largest part comes from USA (11%) and Germany (11%), France (10%), Spain (7%) and United Kingdom (6%), followed by Switzerland, Netherlands, Japan, etc.

HPC - Scientific Computing and Technical Computing

117 Virtual Machines
on HPC Cloud



European data management infrastructure
552 Tb
13.700 K files
6.000 K user access

FORTISSIMO
HPC Cloud for technical computing
and innovation for industries.
14 projects ongoing
5 projects started
1.530 K cpu hours in started projects

Human Brain Project
70 Tb
1.800 K files

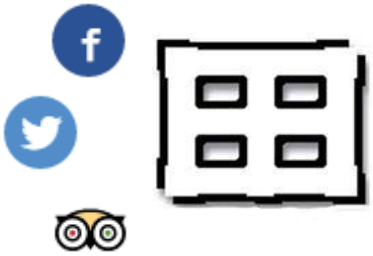
Weather forecast

	2015		2016
Model resolution:			
Step 1	7.0 Km	→	5.0 Km
Step 2	2.8 Km	→	2.2 Km
Day Nodes:	12	→	110
Area:	Italy	→	Mediterranean

Big Data – Bioinformatics

15.000 genomic sample analysed
1.000 Whole Exome Sequencing
6.000 Chip-seq samples
132 users, 55 projects,
4.197 K cpu hours, 179 Tb

Big Data – Analytics



17.000 Fb posts 25.000 tweet 3.000 reviews
7.500 Fb users 10.500 Twitter users
43.000 interactions with social media (6 months)
→ 227.000 terms analyzed on Caserta Royal Palace

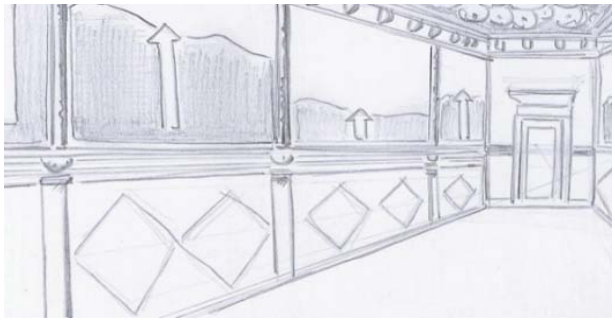
13.000 viewers
1.440 audience data (1 year)
→ 6.832.800 K audience data analyzed!

5.505 K vehicle operating parameters analyzed form on-board diagnostic devices
1.542 K GPS data integrated in the analysis
(Fortissimo PRESERVE project)

20.000 queries on Agriturism
30.000 web sites
→ 20.000 K web pages analyzed

Big Data – Humanities

14.087 render hours
47.776 frames – 34 GB
(Isabella D'Este Virtual Studiolo)



469.293 Metadata records about Contributors
84.143 Metadata records about films
26.195 K Metadata records about Contributors from VIAF
(data coming from 9 European Film Heritage Institutions imported in the the FORWARD catalogue)

6369 Open access datasets
3044 Closed access datasets
1290 Reserved access datasets
763 Under embargo datasets
(Opentesi: Datasets of PH.D Doctoral Thesis coming from 8 Italian Universities)

Presentation of the Users' Reports

Starting from 2012, Cineca is one of the hosting sites of PRACE infrastructures. Indeed, it hosts one of the PRACE Tier-0 systems. Until mid 2016 our Tier-0 machine was FERMI IBM BG/Q system, that, with a computational power of about 2 PF, in 2012 was ranked at position 7 in the list of top 500 supercomputers (https://www.top500.org/). Starting from July 2016 FERMI was replaced by the new Marconi Lenovo NextScale system. This new system is currently the most powerful supercomputer in the European Union, and when it will be completed (mid 2017), it will reach an aggregated computational power of about 20 PF (10 times the power of our old Tier-0 system).

Currently the Cineca HPC infrastructure is accessible mainly through three different competitive calls: PRACE, ISCRA and LISA.

During the last years the most relevant part of our computational resources was assigned at European level through PRACE competitive calls. PRACE systems are available to scientists and researchers from academia and industry from around the world through 2 forms of access:

• Preparatory Access is intended for short-term access to resources, for code-enabling and porting, required to prepare proposals for Project Access and to demonstrate the scalability of codes. Applications for Preparatory Access are accepted at any time, with a cut-off date every 3 months.

• Project Access is intended for individual researchers and research groups including multi-national research groups and can be used for 1-year large production runs, as well as for 2-year or 3-year (Multi-Year Access) production runs. A project access assigns a minimum of 15 Million of core hours on Marconi system, and is intended for the most ambitious and promising HPC scientific projects in Europe.

At the same time researchers with Italian affiliation can have an access to our infrastructure through ISCRA and LISA projects (only if they are base in Lombardy) . The Italian SuperComputing Resource Allocation (ISCRA) releases two kind of call for proposals:

• Class B projects are received twice a year. They under go a peer-review evaluation and a 3-6 months delay is expected before your project gets access to HPC resources. A "Class B" project requests up to 2Million total CPU hours on MARCONI. The typical request is expected to be around 1Million hours and at least require 1024 processors.

• Class C projects are received through continuous submission and reviewed once per month. An average period of about 15 days is required for activating the project. A "Class C" project requests up to 200 Thousand core-hours on the Tier-0 system (MARCONI) and up to 200 Thousand core-hours on the Tier-1 system (Galileo).

Both PRACE, ISCRA and LISA allocate resources on the basis of a peer review process. In both cases the selection is based only on scientific merit, taking into account originality , innovation potential, scientific excellence, qualification and competence of the applicants, international and national relevance of the projects and the match between requested resources and the objectives of proposals. No preliminary allocation between disciplines or provenience is made and a strictly fair peer-review system is implemented.

SuperComputing Application and Innovation (SCAI) team invests a considerable part of his human resources to help researchers to optimize their code for running our HPC systems in order to ensure the best exploitation of our machines. SCAI team also offers support to the Italian scientific community in writing HPC proposals in order to increase their effectiveness.

Both these activities are in agreement with one of the main missions of SCAI department: enabling researchers to solve the scientific challenges of their domain, focusing only on science while benefiting of the extensive experience and specialized skills of our staff.

In the next pages we are pleased to offer you a selection of the scientific reports that each Cineca user has to provide in order to share and disseminate the outcomes of his research activity. The report include both the results obtained from some PRACE and ISCRA projects.

Massimiliano Guarrasi
Cineca

Prace - projects on Fermi


ISC
Condensed Matter Physics
Computational Fluid Dynamics
1.400.000
Valentina Tozzini, NEST - Scuola Normale Superiore
Flexoelectricity in naturally corrugated graphene: a DFT study
1.059.300
Sandro Sorella, Dipartimento di Fisica
High temperature superconductivity by quantum Monte Carlo: the iron-chalcogenides family
958.214
Maurizia Palummo, Department of Physics
Polytypism in Group III-V and IV nanowires: an ab-initio perspective
1.100.000
Marco Micciarelli, SISSA
Color and optical properties of cyanin dye in water solution.
1.775.857
Rita Magri, Dipartimento di Scienze Fisiche Informatiche e Matematiche
UNderstanding extended and point DEFEct interactions AT surfaces from ab-initio quantum approaches
1.432.104
Conor Hogan, Department of Physics
Characterization and control of 2D-nanostructures
400.000
Konstanze Regina Hahn, Department of Physics
Thermal conductivity and boundary resistance in nanostructured graphene
878.000
Luigi Giacomazzi, DEMOCRITOS
(DEmocritos MOdeling Center for Research In aTOmistic Simulation)
Origin and interconversion MEchanims of point defects in Ge-doped silicA based FIBers
200.394
Alberto Debernardi, U.O.S. di Agrate Brianza
2Dimensional H-passivated Si-Ge Heterostructures
446.743
Luciano Colombo, Dipartimento di Fisica
Thermal REctification Without Interfaces: a proof-of-concept computer experiment
2.000.000
Cláudia Cardoso, Centro S3-nanoStructures and bioSystems at Surfaces
Substrate-induced Polarization and Hybridization Effects in Supported Graphene Nanoribbons
1.454.821
Giovanni Cantele, CNR-SPIN - UoS Napoli
Ab-initio DESIgn and characterization of emerging two-dimensional heteROstructUres for technological applicationS
760.000
Marco Bernasconi, Department of Materials Science
Atomistic simulations of thermal transport in phase change nanowires
1.355.450
Valerio Bellini, consiglio nazionale della ricerca
Co Nanostructures on magnetic substrates
909.312
Matteo Barborini, Centro S3 (nanoStructures and bioSystems at Surfaces)
Scanning tunneling spectroscopy through Quantum Monte Carlo calculations
1.966.080
Francesco Zonta, DIEGM
Simulation of geological carbon dioxide sequestration
1.208.333
Alessandra Nigro, DIMEG
Implicit high-order time Integration schemes for a Discontinuous Galerkin method apptied to DNS and ILES of turbulent flows
1.800.000
Emanuele Martelli, Dip. di Ingegneria industriale e dell'informazione
Separation Shock Characteristic Frequencies in Overexpanded Rocket Nozzles
950.361
Anupam Gupta, Dipartimento di Fisica
COMPlex Fluid-Dynamics with nanofluidic DROPlets
643.451
Chiara Galletti, Dip. di Ingegneria Civile e Industriale
Micro-mixing of complex fluids
1.400.000
Matteo Bernardini, Department of Mechanical and Aerospace Engineering
Active COntrol of shock wave Boundary layer Interaction


Life Science – Computational biology
200.000
Aldo Casaleggio, CNR
3-Dimensional Cardiac Arrhythmia Modeling and Simulation
1.400.000
Gianluca Lattanzi, Dipartimento Interateneo di Fisica
Design of Efficient Nanosensors: a Molecular Dynamics Investigation of Porcine Odorant Binding Protein Chemoreception
1.083.848
Giuseppe Felice Mangiatordi, Dipartimento di Farmacia
Exploring molecular mechanisms in AQP4 water regulation
Particle Physics
1.500.000
Massimo D'Elia, Department of Physics
Curvature of the Pseudocritical Line of Strong Interactions: Towards the Continuum Limit
1.712.598
Massimo D'Elia, Department of Physics
Fluctuations of conserved charges of strongly interacting matter
1.420.064
Leonardo Giusti, Dipartimento di Fisica
Topological susceptibility in large-N Yang–Mills theory
1.200.100
Michele Pepe, Sezione di Milano-Bicocca
Equation of State of the gluon plasma
Astrophysics and Plasma Physics
1.161.133
Gianluigi Bodo, Osservatorio Astrofisico di Torino
Fully Convective Accretion Discs with variable thermal diffusivity
2.000.000
Francesco Califano, Dipartimento di Fisica
Dynamo in a Collisionless Plasma
1.771.482
Carmelita Carbone, Osservatorio Astronomico di Brera
Dark Energy and Massive Neutrinos II
1.695.740
Riccardo Ciolfi, Universita' di Trento
Magnetized binary neutron star mergers and early post-merger evolution
1.400.000
Wolfgang Kastaun, Trento University
Structure and dynamics of spinning neutron star merger remnants
1.112.152
Simone Landi, Dipartimento di Fisica e Astronomia
Hybrid 3D simulations of turbulence and kinetic instabilities at ion scales in the expanding solar wind
1.280.068
Andrea Mignone, Unito
Three Dimensional Reconnection in Jets
1.695.244
Antonino Petralia, Physics and Chemistry Dept.
3D MHD modeling of erupting coronal loop flows
Computational Chemistry
600.000
Luca Bellucci, Centro S3
Amyloid peptide at graphene/water interface
200.000
Stefano Fabris, DEMOCRITOS
(DEmocritos MOdeling Center for Research In aTOmistic Simulation)
Ab-initio modeling of novel fuel-cell electrocatalysts under operative conditions
1.200.000
Matteo Maestri, Dipartimento di Energia
First-principles assessment of the support-metal interaction in the catalytic activation of CO2
1.302.904
Federico Totti, Chemistry Dept.
Assessment of Chemical Tailoring of a [Fe4] series on Gold
Computational Engineering
1.228.800
Ilario Mazzieri, MOX - Mathematic Dept.
Physics-based earthquake scenarios for hazard assessment in densely urbanized areas
RA

Eulerian and Lagrangian Turbulence under Strong Rotation

Turbulence under rotation is a paradigmatic problem involving complex physics and complex flow behavior. In presence of high rotation speed, i.e. low Rossby number, the flow tends to become more and more 2-dimensional, being dominated by the presence of strong large-scale coherent structures aligned along the rotation axis. The transition from fully 3D to 2D regime is triggered by the presence of a non vanishing inverse energy flux, as in a pure 2D flow. We have performed a world-record simulation with a resolution up to 4096^3 collocation points, using state-of-the-art pseudo-spectral solver. We have analyzed both the case of weak anisotropy (only forward energy cascade) and strong anisotropy (with forward and inverse cascades), with the assessment of isotropic and anisotropic scaling properties of both the 2D mean field averaged along the rotation axis and the underlying 3D turbulent fluctuations.
The main novelty of our simulation is the advection of millions of light and heavy point-like particles by the rotating flow. The trajectory x and the velocity $v(x,t)$ of a small sphere of radius a and density ρ_p suspended in the fluid field u are:

(1)
$$\frac{dx}{dt} = v$$

(2)
$$\frac{dv}{dt} = \beta\left[\frac{2}{3}\frac{Du}{Dt} + \frac{1}{3}\frac{du}{dt}\right] - \frac{1}{\tau_p}(v-u) - 2\boldsymbol{\Omega}\times(v-\beta u) - (1-\beta)\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times r)$$

The dynamics is controlled by two non-dimensional parameters, the density ratio, $\beta = 3\rho_f/(\rho_f + 2\rho_p)$, and the Stokes number, $St = \tau_p/\tau_\eta$, defined as the ratio between the particle relaxation time, $\tau_p = a^2/3\beta\nu$, and the Kolmogorov time, τ_η.

The term $Du/Dt = \partial u/\partial t + u\cdot\nabla u$ is the fluid acceleration, while du/dt is the derivative of the fluid velocity along the particle trajectory. At variance with the rotating Navier-Stokes equations for the fluid velocity field, the centrifugal force $(\beta - 1)\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times r)$ is explicitly present in the equation for the particles. Its sign depends on the factor $(\beta - 1)$: For heavy particles $(0 \le \beta < 1)$ the force is centrifugal, while for light particles $(1 < \beta \le 3)$ is centripetal. The presence of cyclonic structures (see Fig. 1) is key also for the dispersion and advection of inertial particles. Our simulation presents the first systematic investigation of dispersion of tracers, light and heavy particles in rotating turbulence, at high resolution and with a high number of particles trajectories. Both single particles quantities (acceleration, Lagrangian velocity structure functions) and two-particles quantities (Richardson dispersion) are studied, together with conditional statistics with respect to the underlying flow structures (preferential concentration).

Luca Biferale, Fabio Bonaccorso
Department of Physics and INFN, University of Rome Tor Vergata

Acknowledgement
The numerical study has been performed under the PRACE grant No Pra092256. Part of the numerical data are stored under the EUDAT project TURBASE-DNS.
This study has been funded by the European Research Council under the European Union's Seventh Framework Programme, ERC Grant Agreement No 339032.

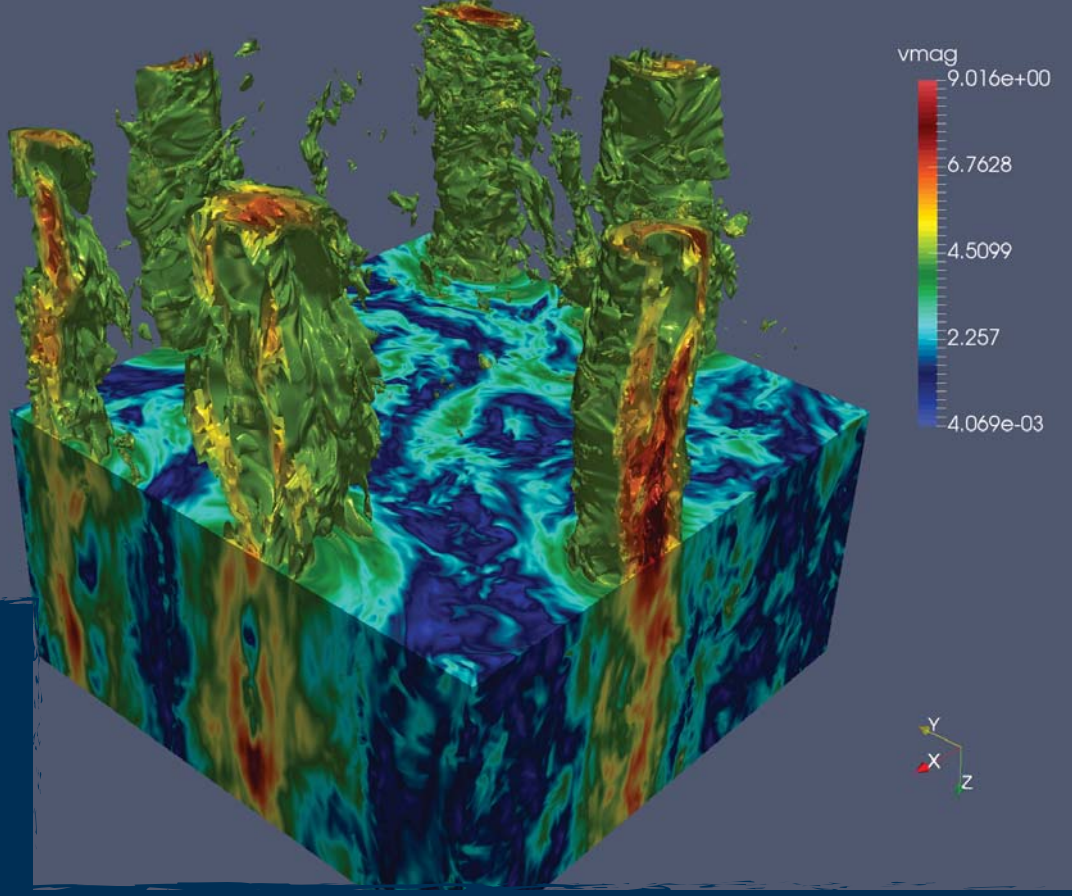


Figure 1
3D rendering of the intensity of the velocity field under strong rotation. Notice the formation of three strong 2D columnar vortices oriented along the rotation (vertical) axis in a fully 3D turbulent background

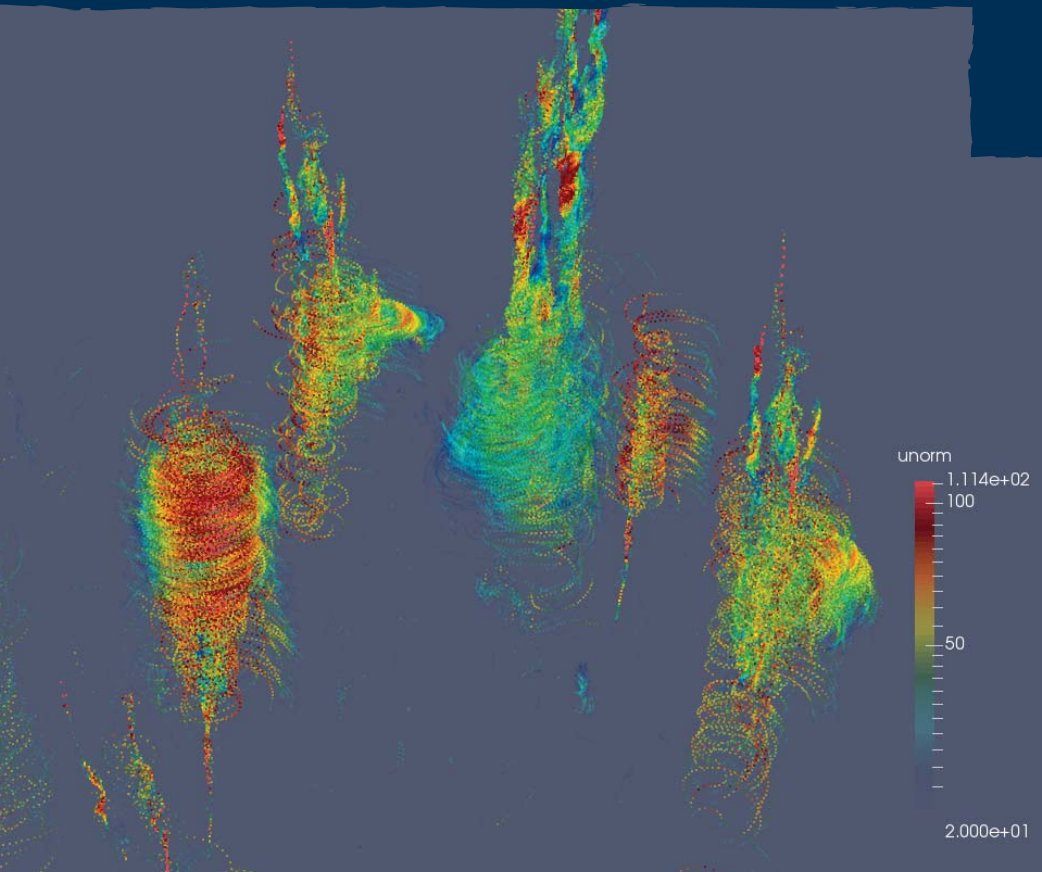


Figure 2
Rendering of trajectories of light particles injected in the flow.

Mixed convection in channel flows with unstable stratification

We study turbulent flow in a planar channel with heating at the lower wall, which introduces unstable stratification owing to buoyancy effects. The goal is to study the interplay between buoyancy and shear, which can yield strong turbulence intensification with incurred heat and momentum transfer enhancement. Mixed convection is relevant in engineering applications of heat transfer, as well as in atmospheric flows. Unstable stratification in the Earth atmosphere is known to be responsible for the formation of large and persistent roll eddies, whose main manifestation are street patterns of cumulus clouds with typical spacing of 2-3 km. In models of global atmospheric circulation, correct modeling of unstable stratification processes is crucial, for instance to properly predict the amount of rain precipitation in the monsoon season. The flow under scrutiny is characterized by two parameters, namely the bulk Reynolds number (Re_b=2 h u_b/ ν, with u_b the mean flow velocity, 2 h the channel height, and ν the fluid kinematic viscosity), and the bulk Rayleigh number (Ra=8 h^3 β g ΔT/($\alpha\nu$), with β the coefficient of thermal expansion, g the gravity acceleration, ΔT the temperature difference between the two walls, and α the thermal diffusion coefficient), measuring the intensity of convection and buoyancy, respectively. Direct numerical simulations (DNS) have been carried out in the range of flow parameters 0<Re_b< 31623, 0<Ra<10^9, with resolution of up to 6144 x 768 x 3072 grid points. Representative results are shown in the attached figure for the case of pure buoyant flow at Ra=10^9 (panel a), and mixed convection at Re_b=31623, Ra=10^9 (panel b), where temperature contours are shown (red denotes high- temperature fluid, blue low-temperature fluid). In the absence of shear the flow near the hot wall wall (x-z plane) organizes itself into a network of high-temperature plumes protruding from the thermal boundary layer into the bulk flow. In wall-normal planes (both x-y and y-z) the temperature contours highlight the formation of large-scale columns of light fluid emerging from the hot wall and downdrafts of heavy fluid descending from the cold wall, which provide hint for the formation of a large-scale circulation. As bulk convection is introduced (panel b) the temperature in the near-wall plane still exhibits a network pattern, but plumes are now clearly aligned along the streamwise (x) direction, and they clearly undergo spanwise undulation and distortion induced by strong secondary motions. Large-scale ascending and descending motions are still apparent in cross-stream (y-z) planes, whereas an organization closer to that observed in pure shear flows is observed in x-y planes. These are the symptoms of the formation of longitudinal rollers spanning the full channel thickness, and which we have found to form owing to the interplay of convection and shear in a wide range of flow parameters. Analysis of flows in the full parameter space has led to characterize the universal behavior of the mean velocity and temperature profiles, as well of their fluctuation intensities in light of the Monin-Obukhov (MO) theory. While the DNS generally confirm the MO parametrizations resulting from field experiences (which by the way are subject to a large degree of scatter), significant deviations from the alleged trends are found in the light-wind regime, which if confirmed would open the pathway for improved models of global atmospheric circulation.

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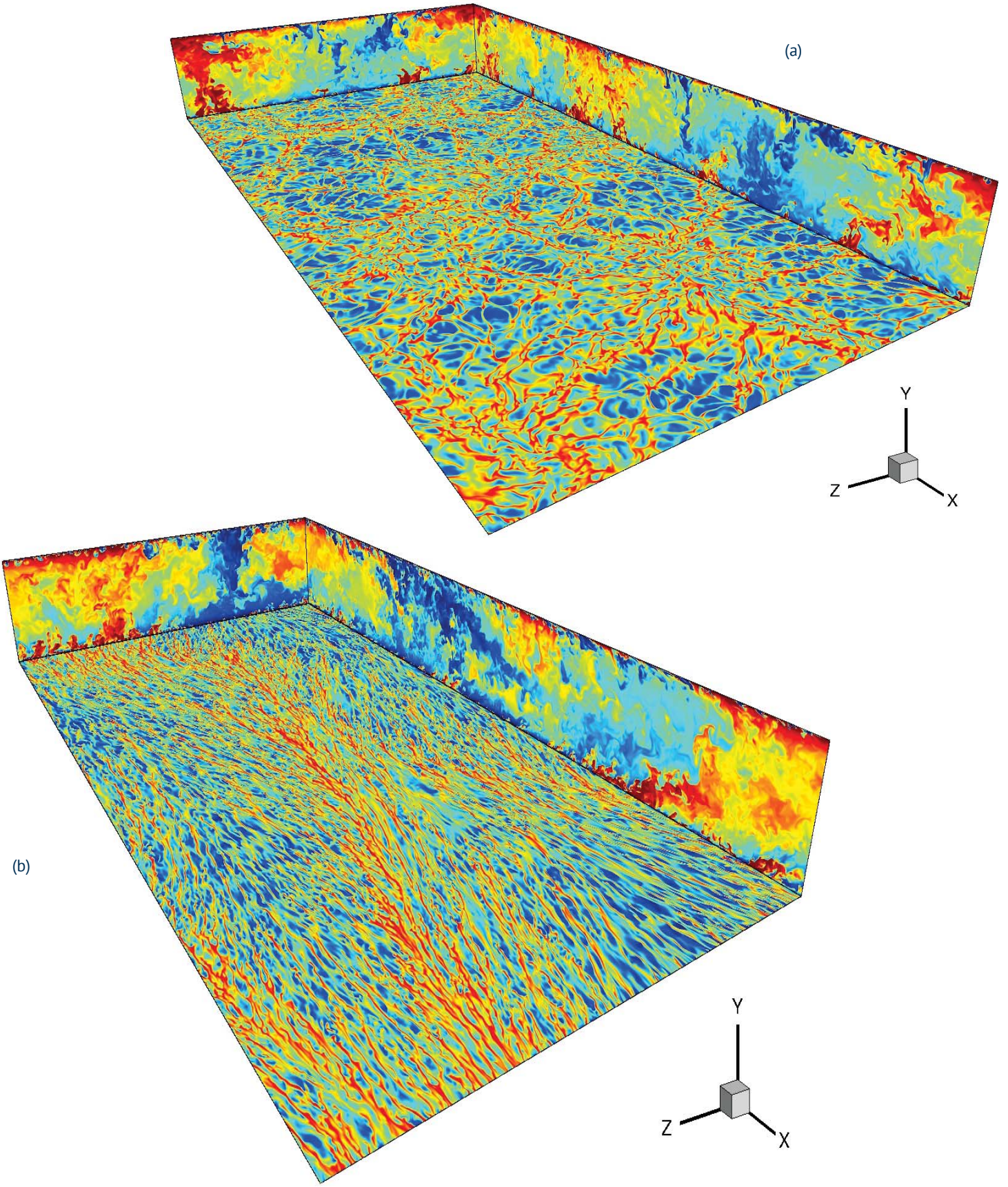
(a)
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Salvinia-inspired surfaces for underwater superhydrophobicity

Superhydrophobic surfaces show promise to control important flow and wetting characteristics through chemical and topographical structuring of surfaces at the micro and nanoscale. Many interesting properties, such as self-cleaning, enhanced liquid repellence, and drag reduction are linked to the suspended Cassie state, in which gas bubbles are entrapped within surface roughness (Figure 1). The Cassie state is sustained by the capillary forces that are dominant on the typical scales of surface roughness. However, depending on the pressure and temperature of the system, the Cassie state can be metastable or stable. On the other hand, if the liquid wets the whole surface (Wenzel state) superhydrophobicity is lost. The central problem of superhydrophobicity is therefore the Cassie-Wenzel transition.

In recent years, bioinspiration played a major role in designing artificial surfaces with tailored wetting properties. While the first theoretical and experimental investigations focused on the properties of drops on superhydrophobic surfaces being inspired by the Lotus leaf, a growing body of literature is concerned with the properties of submerged surfaces. The main reason for this increasing interest is that superhydrophobic coatings show promise for underwater drag-reduction[1]; such applications, however, require durable gas domains resisting to large pressures. The most intriguing natural example of durable underwater gas-trapping is the Salvinia molesta; the leaves of this infesting water fern evolved topographically and chemically complex hairs that allow the plant to preserve a gas layer under extreme environmental conditions see Figure 1 and Ref.[2]. The structure of these hairs resemble an egg-beater and they are covered with a hydrophobic wax but on their tip, where a small hydrophilic patch is present.

This research aims at understanding of the stability of the Cassie state induced by complex (bioinspired) surface textures in submerged conditions, i.e., at different pressures. There are two main computational challenges in this project. The first is dealing with three-dimensional structures and complex chemical properties which require simulating large systems. This computational effort allows to reproduce more closely surfaces of technological relevance. In particular, we are interested in investigating "collective" wetting phenomena involving more than one cavity, such as zipping transitions. Such phenomena are frequent when dealing with interconnected gas domains typical of engineered structures. The second numerical challenge is related to rare events in the wetting and dewetting process of rough hydrophobic surfaces: the presence of multiple metastable states separated by free-energy barriers much larger than the thermal energy calls for dedicated, computationally intensive techniques for effectively sampling the phase space.

Rare events molecular dynamics simulations were carried out on 2D systems reproducing the salient features of the Salvinia molesta (Figure 1) and on 3D pillared structures (Figure 2) using Cineca supercomputers FERMI and MARCONI granted through PRACE projects 2013081560 and 2014112591, ISCRA B HP10BK123U, and ISCRA C HP10CUBCMI. Results have helped understanding the physical reason of the "Salvinia paradox"[2]: 1) the hydrophobic re-entrant geometry of the hairs hinders the collapse of the gas pockets when subject to large hydrostatic pressures; 2) the small hydrophilic patches prevent gas to escape as a consequence of bubble nucleation at pressures below the equilibrium vapor pressure[3,4,5]. This simulation campaign culminated in the formulation of design principle for achieving robust underwater superhydrophobicity[3].

The ongoing simulation campaign on 3D textures has highlighted a collective wetting mechanism, involving several interpillar-spacings at the same time. Furthermore, many fundamental challenges emerged during this simulation campaign: several rare event methods - the string method and restrained molecular dynamics - were compared, finding that the description of the thermally activated wetting process in terms of a single "collective variable" is insufficient: only the density field yields consistent results (cf.[6]).

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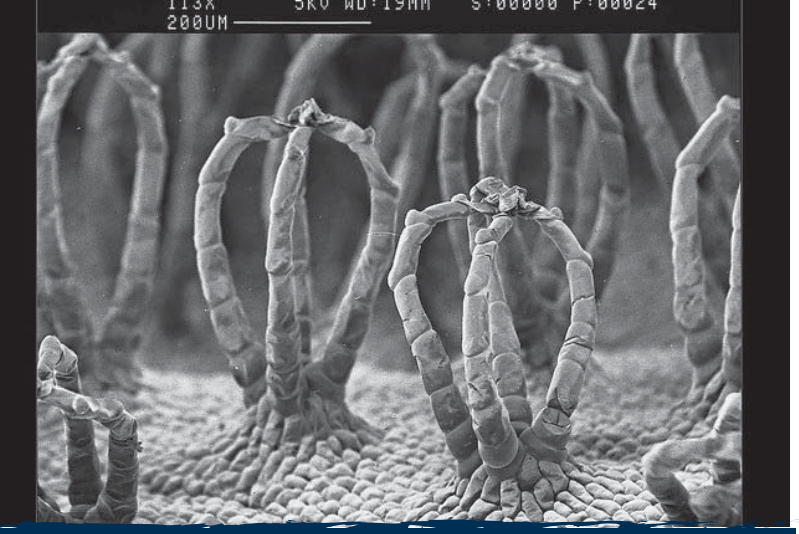
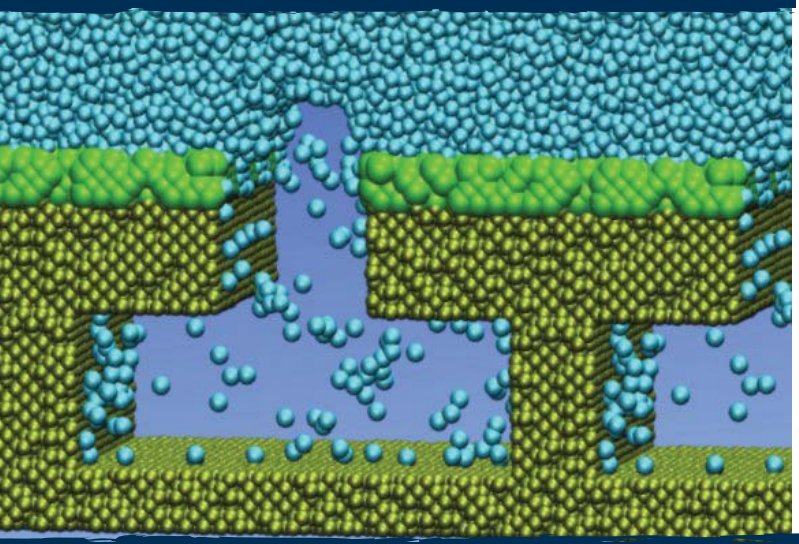


Figure 1
Upper) Micrograph of the Salvinia molesta leaf, showing the egg-beater-shaped hairs with a hydrophilic patch on top (copyright W. Barthlott, Lotus-Salvinia.de).
Lower) Atomistic system mimicking the Salvinia: the light green particles are hydrophilic while the dark green are hydrophobic.



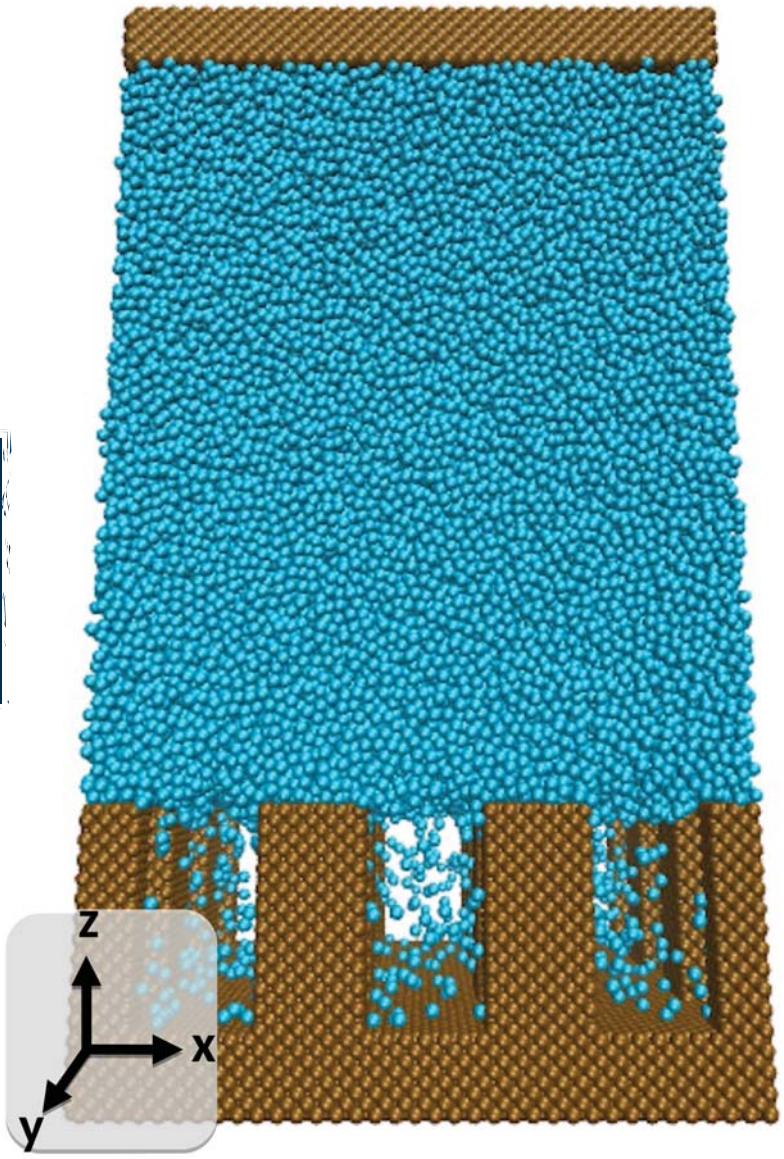


Figure 2
Capturing the wetting mechanism of 3D arrays of pillars requires simulating large systems.

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Hybrid 3D simulations of turbulence and kinetic instabilities at ion scales in the expanding solar wind

Turbulence in magnetized collisionless plasmas, such as the solar wind, is one of the major challenges of space physics and astrophysics. Both the anisotropic flow of energy toward smaller scales (cascade) and the damping of energy at dissipative scales are poorly understood. In a turbulent cascade, fluctuations at a large driving scale contain most of the energy, but there is energy transfer to fluctuations with smaller and smaller scales. The dissipation of turbulent fluctuations operates at scales where particle kinetics dominates. In-situ measurements in the solar wind represent a unique opportunity to study those processes, since they provide observations in a huge range of scales. The estimated turbulent energy cascade rate is comparable to the proton heating needed to explain the non adiabatic evolution of the solar wind plasma during its expansion. This suggests that turbulence plays an active role in transferring energy from electromagnetic fields to particles and heats the solar wind plasma. However, the processes that ultimately lead to heating in a collisionless turbulent medium are still unknown. This study intended to apply 3D hybrid particle-in-cell (HPIC) simulations to understanding how astrophysical turbulence operates and how plasma properties control or react to its evolution. Our recent 2D numerical studies[1,2] showed the HPIC approach to represent a very efficient and reliable methodology for investigating this topic over a wide range of scales, being able to recover many properties of solar wind observations. A 2D geometry may in principle strongly constrains numerical results, by affecting the propagation of modes, inhibiting the presence of small-scale parallel waves, constraining possible competing mechanisms (e.g., instabilities) and limiting the shape and size of dissipative structures. Therefore, 2D results need to be verified with more realistic 3D simulations employing a high accuracy, i.e., millions of grids points and hundreds of billions of particles, so the use of thousands of cores and many TBs of memory on large HPC systems is essential.

We performed a state-of-the-art simulation of strong decaying turbulence in presence of a guide field, with an intermediate value of the plasma beta (ratio of the plasma pressure to the magnetic pressure) $\beta = 0.5$, employing a very similar setup and similar parameters of the 2D simulation presented in[1,2]. It employed a 512^3 computational grid and 2000 particles-per-cell, for a total of 270 billions particles. A preliminary analysis shows:

i) the sudden formation of a large spectral anisotropy, despite the isotropic initial condition [Figure 1, 2],

ii) the development of a turbulent cascade that mainly develops in the direction perpendicular to the mean field [Figure 1, 2],

iii) a double power-law behavior over almost two decades in wavenumber in the isotropized 1D magnetic field spectrum, with an ion-scale break separating a -5/3 slope at large scales from a ~-2.8 slope at sub-ion scales [Figure 3],

iv) a coupling between density and magnetic fluctuations at sub-ion scales [Figure 3].

Although the magnetic structures look quite different in real space in respect to the 2D case, since clear coherent structures, e.g., vortices and magnetic islands, are not identifiable, the spectral properties show a very good qualitative and quantitative agreement. The preliminary analysis of the 3D results strongly validate our 2D previous studies.

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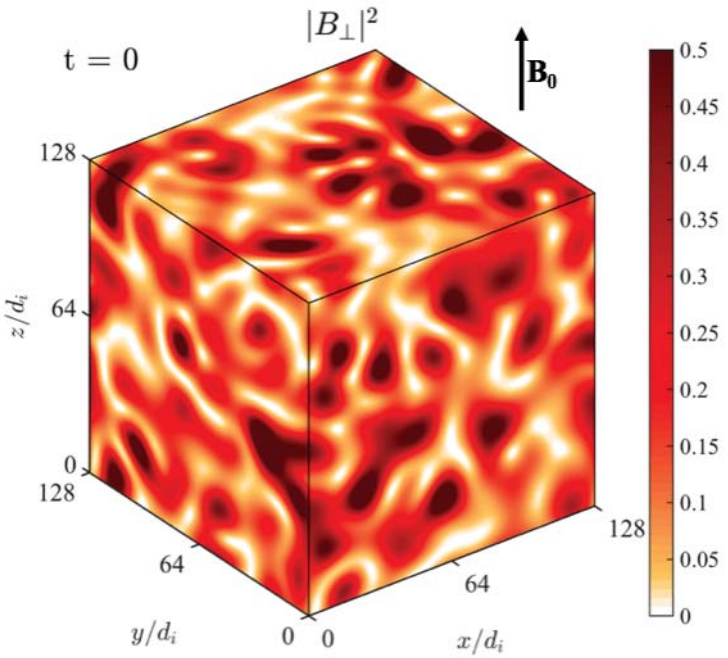
Acknowledgments

This project was supported by a PRACE program (HybTurb3D).



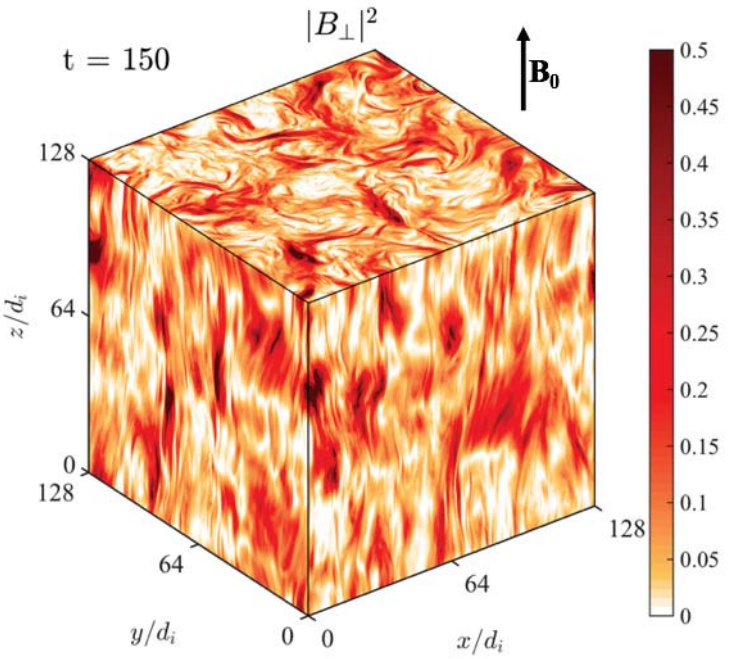


Figure 1
Amplitude of the magnetic fluctuations perpendicular to the ambient magnetic field at t=0 (left) and at a time when turbulence is fully developed (right).

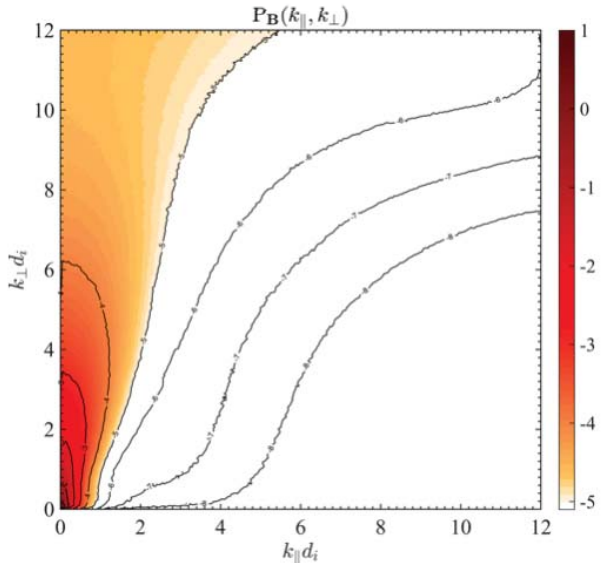
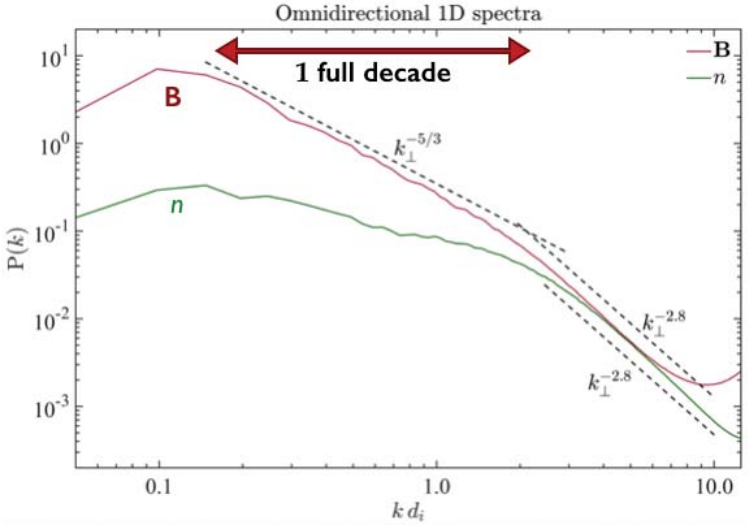
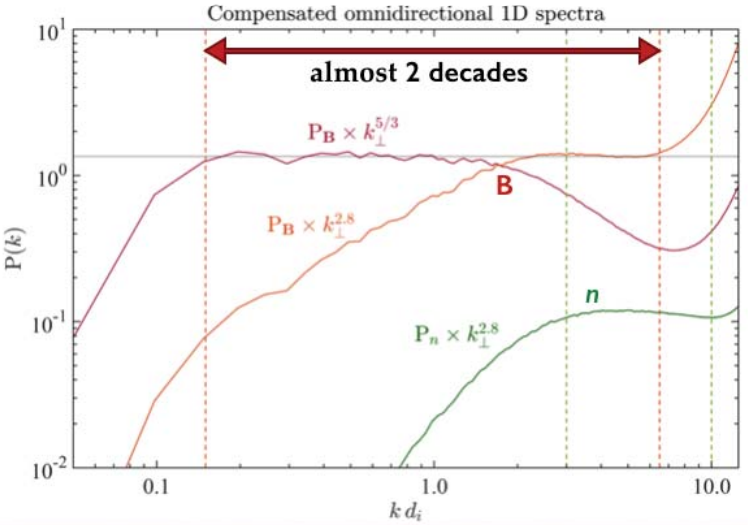


Figure 2
Two-dimensional power spectrum of the magnetic fluctuations versus the parallel and perpendicular wavenumbers with respect to the ambient magnetic field.

Figure 3
Left panel: Omnidirectioanl one-dimensional power spectra of the magnetic (red) and density (green) fluctuations from large-fluid scales until small-kinetic scales. Right panel: the same as in the left panel, but the spectra have been compensated by precise powers of the perpendicular wavenumber.





Spray formation: a numerical closeup

We solve the Navier-Stokes equations for incompressible flow with sharp interfaces and constant surface tension using the free (GPLv3) multiphase flow solver, ParisSimulator, and conducted simulations of atomization in the two-phase mixing layers as in the experiment of Matas et al. 2011 (Phys. Fluids, 23:094112, 2011). In a large three-dimensional box $L_x \times L_y \times L_z$ dimensions, we inject gas and liquid streams through the boundary x = 0, which are separated by a solid plate with dimensions $l_x \times e \times L_z$. There is a boundary layer of thickness δ on the plate. The thickness of the gas stream is H. The dimensions of the box are L_x = 16H and L_y = 8H while L_z = 2H. The values of the corresponding dimensionless parameters are given in Table 1, using standard notations.

M	r	m	$Re_{g,\delta}$	$We_{g,\delta}$	$Re_{g,H}$
$\rho_g U_g^2/\rho_l U_l^2$	ρ_l/ρ_g	μ_l/μ_g	$\rho_g U_g \delta/\mu_g$	$\rho_g U_g^2 \delta/\sigma$	$\rho_g U_g H/\mu_g$
20	20	20	1000	10	8000

Table 1. Dimensionless parameters of the simulation.

The fields are discretized using a fixed regular cubic grid. The simulations are performed on three grids called M0, M1, M2, M3, so that Mn has $H/\Delta x = 32 \times 2^n$ points in the gas layer. The computational time required for these four simulations are given in Table 2.

Grid	Δx (μm)	H/Δx	Number of Cells	Number of Time Steps	Total CPU Time
M0	25	32	8.4 Million	$4.9\ 10^4$	$2.5\ 10^3$
M1	12.5	64	67 Million	$1.0\ 10^5$	$4.3\ 10^4$
M2	6.25	128	537 Million	$2.2\ 10^5$	$5\ 10^5$
M3	3.125	256	4 Billion	$5.0\ 10^5$	$20\ 10^6$

Table 2. Hierarchy of grids used and the CPU time required for the corresponding simulation.

There are two purposes for this set of simulations: 1) to prove the convergence of simulations at least for large-scale physical quantities such as droplet size distribution; 2) to explore in detail the underlying drop formation mechanisms.

An overview of the atomizing jet on the M3 grid is shown in the figure below. As can be seen the multiphase flow arising from atomization is complex and chaotic, involving a wide range of length scales. Different mesh levels and numerical methods are considered to investigate their effects to the spray formation.

The most important result for which computing power is most needed is the convergence study of the distribution of drop sizes. The converged distribution results are then compared to various predictions and models (e.g., log-normal and Gamma distributions).

Atomization process plays an important role in a broad range of industrial and environmental applications such ocean-atmosphere interactions. For more information see Y. Ling, D. Fuster, G. Tryggvason & S. Zaleski 2016: Spray formation: a numerical closeup. ArXiv preprint arXiv:1511.04234 v2.
http://www.ida.upmc.fr/~zaleski/Papers/spray_form_v8.pdf

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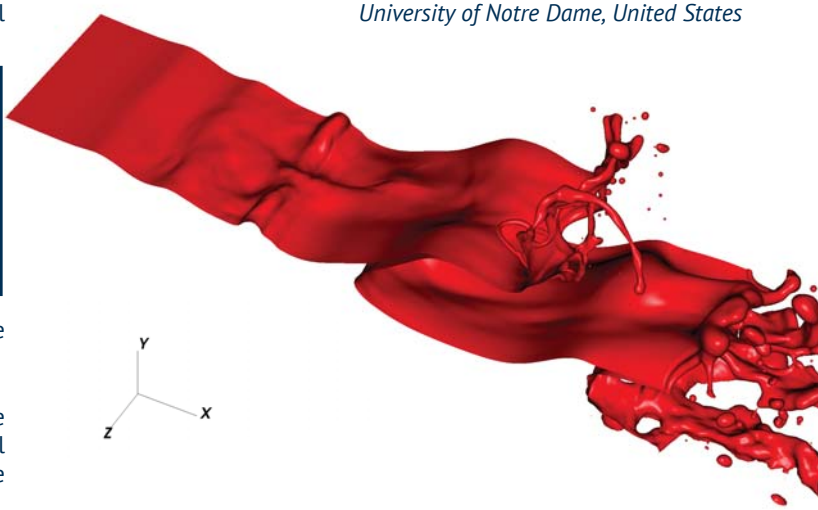

Guided flows in coronal loops

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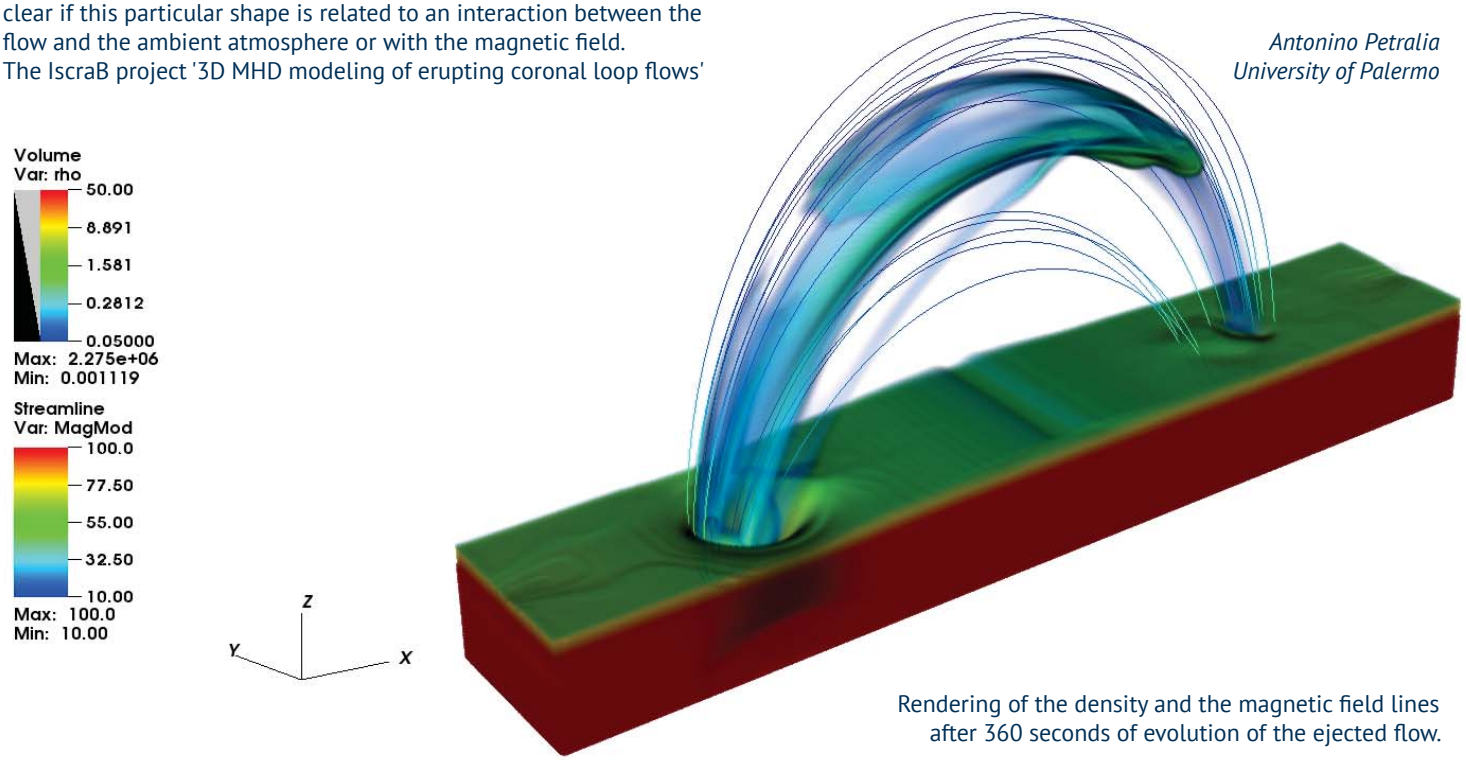
The corona is the outer part of the solar atmosphere, characterized by a gas fully ionized at temperatures greater that one milion degree, interacting with the ambient magnetic field. Because of this interaction, the corona appears structured and bright in EUV and soft-X bands, but also very dynamic. The presence of flows is confirmed by both images and doppler shifts.
Recent EUV observations (e.g. http://www.lmsal.com/hek/her?cmd=view-voevent&ivorn=ivo://helio-informatics.org/ERMET_KarelSchrijver_20151105_214937) showed that many coronal flows are squashed into ribbons. It is not clear if this particular shape is related to an interaction between the flow and the ambient atmosphere or with the magnetic field.
The IscraB project '3D MHD modeling of erupting coronal loop flows' helps to clearify that the initial inclination between the magnetic field and the velocity of the flow is crucial in determining the dynamics of the flow and it can explain the observed features.
We built a 3D MHD model of solar atmosphere immersed in a closed magnetic field with the effect of gravity, thermal conduction, radiative losses. Our computational grid is adaptively refined up to an equivalent cell size of 60 km. We used the 3D-MHD PLUTO code to run the simulations on both 4096 Cineca/Fermi cores and 1080 Cineca/Marconi cores.



Rendering of the density and the magnetic field lines after 360 seconds of evolution of the ejected flow.

ISCRA

The RNA that snips and stitches RNA

Messenger RNA (mRNA) convey genetic information from DNA to the ribosome, where it specifies the amino acid sequence of the proteins. Before reaching its mature form, premature mRNA is made up of exons and introns, which correspond to coding and non-coding portions of genetic information, respectively. Introns have to be "switched off", namely removed from the sequence, while exons have to be joined together to form mature mRNA. In some prokaryotes as well as in the organelles of some eukaryotes, this "snipping and stitching" process, known as splicing, is self-catalyzed by particular ribozymes with the help of magnesium ions. The group II introns ribozymes are in fact able to self-regulate their own removal from the filament, thus promoting the maturation of messenger RNA.

In humans, the splicing process, is governed by a huge machinery consisting of proteins and RNA, the spliceosome, whose "core" has many structural and catalytic similarities with group II introns, according to recent studies. Detailed structural information for this machinery are fragmentary to date, hampering a detailed understanding of its function.

So far, the exact mechanism by which splicing occurs was unknown, but a new SISSA/CNR-IOM study -published on the Journal of the American Chemical Society carried out by Lorenzo Casalino and coordinated by Dr. Alessandra Magistrato and done in collaboration with the École polytechnique fédérale de Lausanne (Dr. G. Palermo and Prof. U Rothlisberger) has elucidated in detail the cleavage process for group II introns by using computer simulations.

Group II introns are considered the ancestors of the spliceosome, thereby this study may shed light on the much more complex splicing mechanism in humans. This article unveiled that, although ribozymes are enzymes made of RNA, catalysis in group II introns occurs in a radically different manner from protein enzymes and thus the mechanism is remarkably different from what had been hypothesized for decades.

This is due to the fact that enzymes use far more specific methods due to the chemical richness of amino acids, whereas the catalytic process in ribozymes adapts to the skeleton of the RNA , resulting in a slightly slower but equally precise reaction mechanism. Given the analogy of group II introns with the central core of the human spliceosome, which is the important portion for splicing, this work can help to guide research and provide a glimpse into the spliceosome mechanism.

The implications of this are enormous: aberrant splicing in humans may lead to various complex diseases and also underlies the development of some forms of cancer and the onset of neurodegenerative diseases, so a better understanding of the process can add important information for our fight against these diseases.

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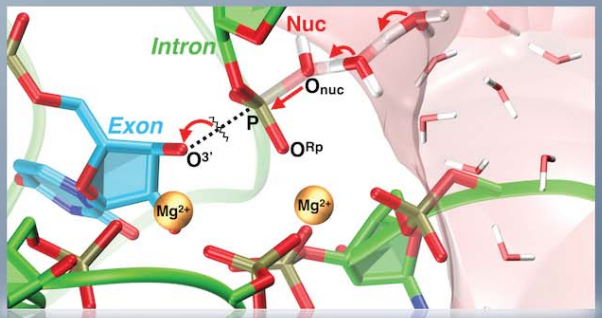
Acknowledgments
This project was supported by an ISCRA B (SpliRNA).

Molecular simulations reveal a novel RNA-specific two-Mg^{2}+-ion mechanism for the splicing reaction of group II intron ribozymes (top-right), the evolutionary ancestors of the eukaryotic spliceosome (top-left), with the bulk water playing an unprecedented role as proton acceptor of the activated nucleophile (bottom). The unveiled splicing mechanism of group II introns sheds lights on the more complicated process occurring in the eukaryotic spliceosome.



ISCRA

Collective dynamics of large droplets in turbulence

Understanding the dynamics of liquid-liquid mixtures is of fundamental importance in a number of industrial and environmental applications.
Important examples include oil-water separators and hydrocarbon transportation pipelines. In these situations, two liquids (typically oil and water) are driven inside confined channels and interact modifying the overall mass, momentum and heat transfer properties of the system.
To optimize the design of these systems it is crucial to determine whether the two phases remain separate (due to density and viscosity stratification) or form emulsions (which are difficult to process/separate).
In many circumstances, due to the underlying large shear stress and turbulence intensities, the oil-water mixtures appear as oil droplets transported by a water carrier flow.
In the present study, we use Direct Numerical Simulation to analyze the dynamics of large deformable droplets dispersed in a turbulent flow. A phase field approach (coupling Navier-Stokes and Cahn-Hilliard equations) is used to describe the liquid-liquid interactions. Droplets have the same density of the carrier fluid, but different viscosity.
In particular, we consider a wide range of droplets-to-fluid viscosity ratio $\lambda = \mu_d/\mu_f$ (with μ_d the viscosity of droplets and μ_f the viscosity of the carrier fluid) ranging from $\lambda = 0.01$ to $\lambda = 100$.
Droplets dynamics is primarily controlled by the interplay between turbulence fluctuations, surface tension (measured through the Weber number We) and droplet-to-fluid viscosity ratio (λ). We specifically focus on the role of We and λ.
In general, droplets can coalesce and break, depending on the value of physical parameters.
Coalescence (Figure 2) happens when two droplets come close and collide due to turbulence fluctuations. During the collision, a small bridge is initially formed; later, surface tension (which tends to restore the spherical shape) comes into the picture and complete the coalescence process.
Break-up (Figure 3) happens when a droplet is subjected to a sufficient shear stress, such that it is deformed and stretched until the emerging thin liquid bridge is broken (due to surface tension that acts minimizing the energy stored at the interface).
Our results also indicate that for small We, droplets are only slightly deformed and their viscosity does not influence the coalescence/break-up rate. For larger We, droplets are deformable and their viscosity can significantly alter the coalescence and break-up dynamics.

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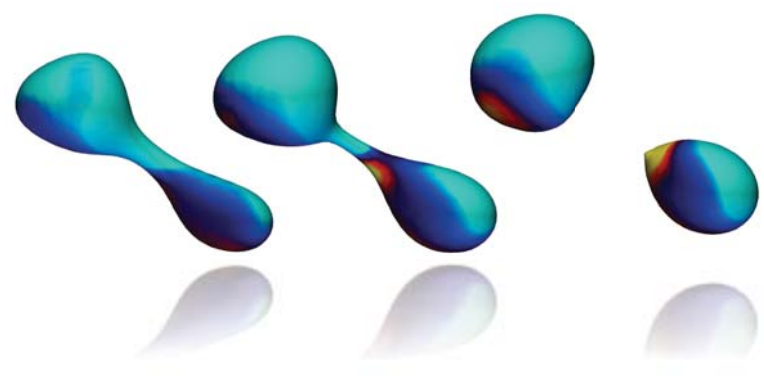
Figure 1
Droplets coalescing and breaking up in turbulence. Flow streamlines are explicitly shown to highlight the complex droplets/turbulence interaction.

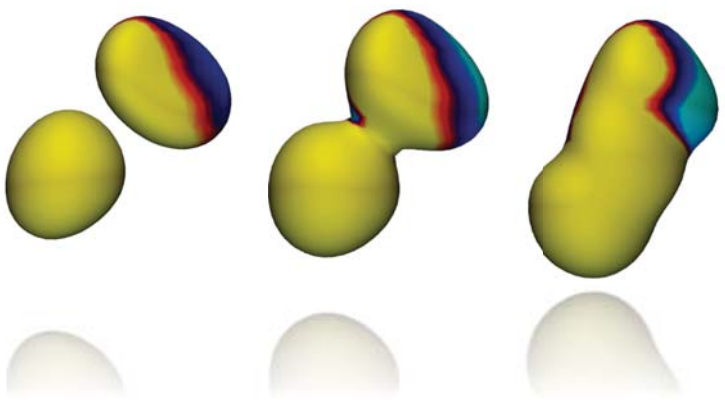
Figure 2
Physics of a coalescence event: two droplets come closer under the action of turbulence fluctuations, until they finally merge. Contours indicate streamwise velocity fluctuations.

Figure 3
Physics of a breakup process: a large droplet is subjected to shear such that it breaks into two smaller droplets. Contours indicate streamwise velocity fluctuations.

BREAK-UP



COALESCENCE



ISCRA

Turbulent dynamo in a collisionless plasma

Magnetic fields pervade the entire Universe and affect the formation and evolution of astrophysical systems from cosmological to planetary scales. How such fields arose in the early Universe, and were further amplified to the dynamically significant levels reported today is a major astrophysics problem.

Many astrophysical systems are in an electrically conducting plasma state and are strongly turbulent. This combination is thought to give rise to dynamo effects, whereby some of the kinetic energy of turbulent motions is converted into magnetic energy. In environments such as stellar interiors where the particles mean free path is much shorter than typical flow scales, one can use a magnetohydrodynamic (MHD) fluid description to describe the coupled evolution of the flow and magnetic field. The fluid dynamo idea dates back to Larmor in 1919, and mathematical theories were developed in the 1960s. However MHD dynamo action was only demonstrated numerically in 1981 in pioneering simulations by Meneguzzi, Frisch and Pouquet. The intrinsic three-dimensionality of the process made it hard to simulate at the time.

What about dynamo in weakly collisional plasmas? For instance, in the hot plasma that makes for 15% of the composition of galaxy clusters, the proton mean free path is of the order of a few kiloparsecs, comparable to the reported typical size of density or magnetic fluctuations. Could cluster magnetic fields have been generated through a dynamo effect powered by weakly collisional turbulence? This question, as well as many others including that of the low luminosity of the surroundings of the supermassive black hole at our galactic centre, cannot be addressed with MHD, and requires a fully kinetic, collisionless dynamical description. For the dynamo problem, this involves solving the Vlasov-Maxwell equations in a six-dimensional phase space plus time — that is, three more dimensions than in MHD! Just five years ago, this looked like a daunting prospect numerically. However, thanks to the advance of computing technology, we have recently been able to perform the first set of collisionless dynamo simulations using about 20 Million hours of Blue Gene/Q CPU at Cineca and IDRIS (France).

Our results establish that a collisionless plasma dynamo is indeed possible, and proceeds on a timescale comparable to the turbulence turnover time, as in MHD. This suggests that micro-Gauss magnetic fields inferred by polarimetric measurements in galaxy clusters may well have been generated through a dynamo effect on cosmologically short (hundred million years) timescales. Besides, our simulations reveal that this dynamo enters a fascinating kinetic magnetized dynamical stage once the magnetic field becomes large enough that the ion Larmor (gyration) radius becomes smaller than turbulent eddies. As the magnetic field gets stretched by the flow, the pressure in the plasma becomes anisotropic with respect to the local magnetic field, resulting in the excitation of Larmor-scale kinetic instabilities known as the mirror and firehose instabilities. These fluctuations become entangled with the larger-scale dynamo-generated field, leading to a compelling spaghetti-plate-like magnetic structure illustrated in the Figure (positive/negative pressure anisotropies are color-coded in red/blue on magnetic-field lines). These various effects are absent in collisional MHD. Understanding the effective dynamical consequences of this "foam" of instabilities for the large-scale dynamical evolution represents a major challenge for the future - and will require even bigger computational resources!

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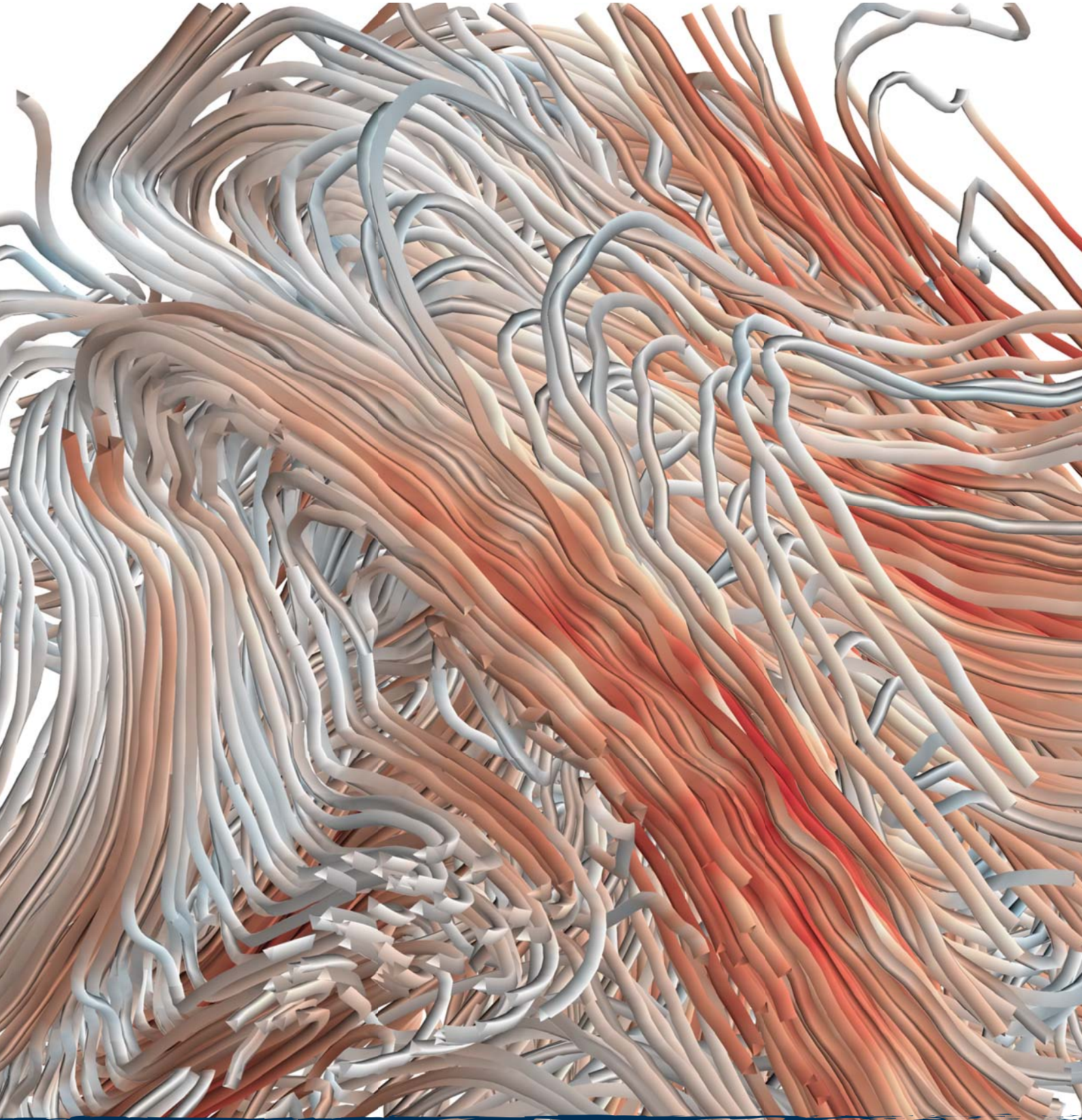

3D rendering of magnetic field lines in a collisionless plasma dynamo simulation, highlighting both the large-scale structure of the dynamo mode and the small-scale structure of parasitic kinetic firehose and mirror instabilities. The colours encode the sign and magnitude of the pressure anisotropy with respect to the local magnetic field direction.

ISCRA

Modeling aided graphene morphing

Graphene displays unique properties, which promise a wide applications range. However, bare graphene is generally not optimal: it has low density of carriers and null band gap, its bidimensionality and low physical-chemical reactivity make it not very effective for gas storage or other volumetric application. Therefore, the capability of manipulating its properties assumes a key role. We explored several aspects of graphene morphing (structural manipulation, chemical-physical decoration, interaction with environmental conditions), with an approach based on a synergistic integration of modeling and experimental data, obtaining results about the relationships between chemisorption, corrugation and electronic properties[1,2].

In the last year we demonstrated that graphene monolayer on SiC has a multi-stable corrugation pattern[3] (Figure 1). Because the reactivity is enhanced on convex areas, this opens the road to the possibility of driving the chemical adhesion of atoms or functional groups[4], aimed at designing graphene based 3D frameworks with specific structural characteristics for gas storage, motion, separation and other functionalities. Our studies indicate that the curvature amplitude and pattern could be controlled by external environmental conditions (temperature, electric fields).

Concerning electronics applications, the "Quasi Free Standing Graphene" on SiC produced by H intercalation in the system (Figure 2) reveals interesting features due to vacancies in the H coverage. Our preliminary results indicate the presence of localized states near the Fermi level[5], which would allow tuning electronic properties of graphene by means of H intercalation control. This work might also clarify some unknown aspects of the H intercalation process, such as the dynamics of formation of hydrogenated domains and the final symmetry of location of the H coverage vacancies. These studies are supported by ISCRA and by EU-H2020 (PRACE, Graphene-Core1 and MCSA)[6].

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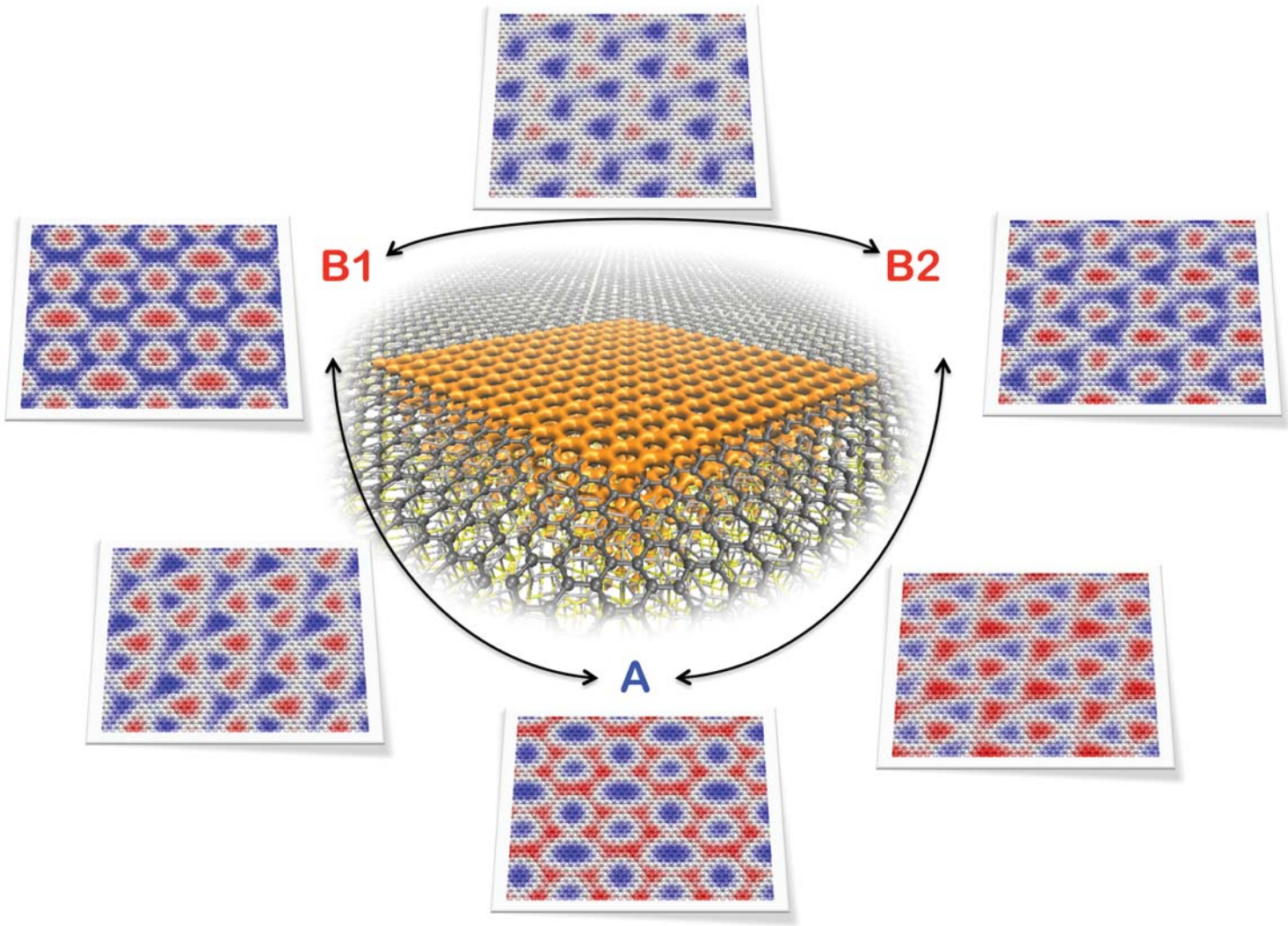
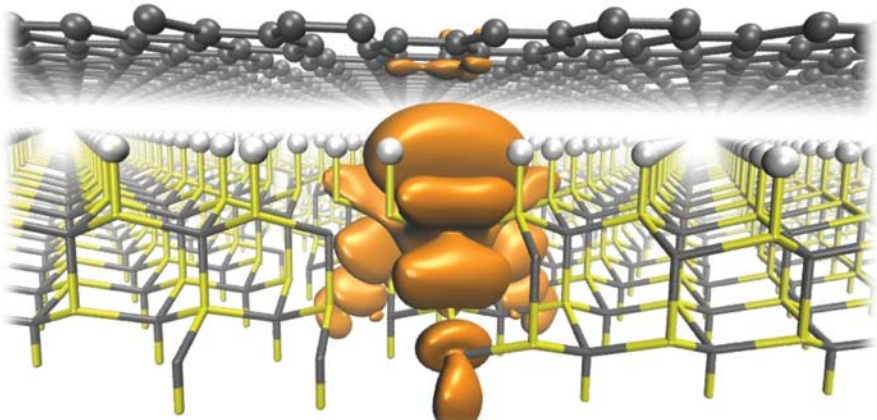
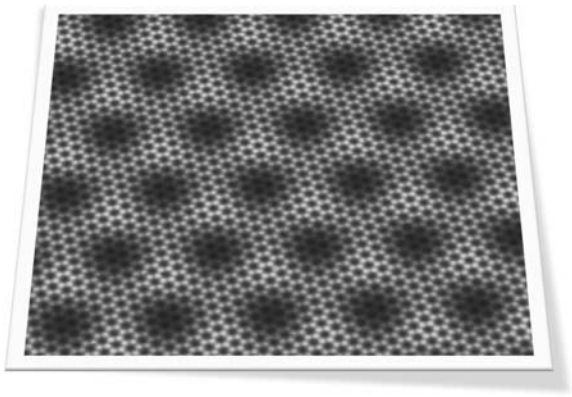


Figure 1
A pictorial representation of the graphene monolayer on SiC. Snapshots represent AFM-like images of the corrugation patterns and transition among them.

Figure 2
A view of the quasi-free standing graphene on SiC with an iso-electronic density surface of the localized electronic state, located on the H vacancy. The snapshot reports an AFM-like image with vacancies located on a regular super-lattice.





ISCRA

Micro-mixing of complex fluids

Efficient mixing in small volumes is a key target in many processes, encompassing miniature fuel cells, molecular diagnostics and, in general, micro-reactors. The simplest micro-device is a T-shape mixer, found as a junction element in more complex micro-systems.
Laminar mixing in such device has been largely investigated when feeding water at the same conditions and flow rates. The inlet streams remain separated up to a critical Reynolds number, corresponding to the transition from a vortex flow regime, presenting a double pair of counter-rotating vortical structures with double-mirror symmetry, to an engulfment flow regime, with a pair of co-rotating vortical structures and central-point symmetry. Further increasing Re, the flow becomes first unsteady and time-periodic, and eventually chaotic.
The practical use of micro-devices involves the mixing of different fluids or of the same fluid at different conditions, so the present project wants to investigate how fluidity of mixing affects steady and unsteady flow regimes in T-mixers. Direct Numerical Simulations of liquid binary mixtures with positive or negative fluidity of mixing (i.e. the mixture viscosity is smaller or larger than that of the pure fluids) were performed using the spectral element code NEK5000. The mixing of water entering at different temperature was also studied as in this case even a small temperature increase of 10 K leads to a drop in viscosity of about 30%. Stability analysis was used to elucidate the mechanisms triggering the onset of the different flow regimes.

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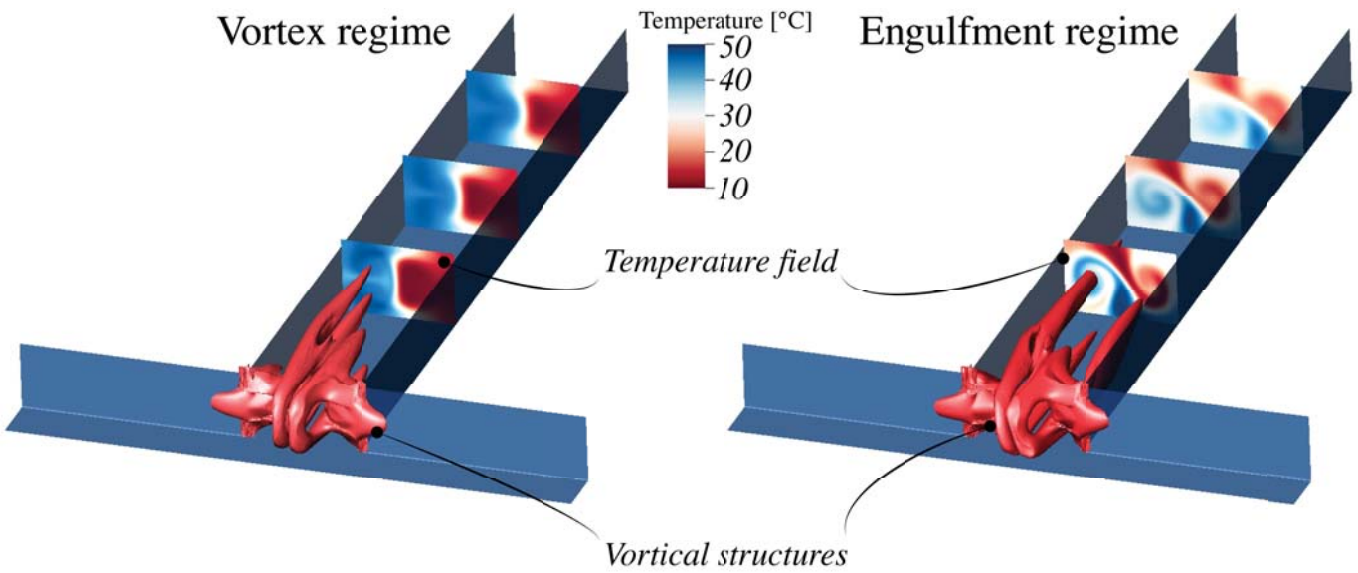

Vortical structures and temperature distribution in vortex and engulfment regimes predictec when feeding water at different temperature into the T mixer. The vortex regime shows a single-mirror symmetry.

ISCRA

Chiral symmetry breaking in QCD Lite

The fundamental theory of the strong interactions in Nature is Quantum Chromodynamics (QCD). One of its crucial properties is the spontaneous breaking of chiral symmetry in the limit of massless quarks. Yoichiro Nambu conjectured this mechanism in the 1960s to explain why the pions as observed in nature are much lighter than other hadrons, an idea for which he was awarded the Nobel prize for Physics in 2008. The mechanism also removes the mass degeneracy of individual hadrons, e.g. the proton, with a partner of opposite parity, which would have to be there if chiral symmetry was not broken.

A distinctive feature of the presence of spontaneous chiral symmetry breaking in QCD is the condensation of low modes of the Dirac operator near the origin as suggested by Banks and Casher[1]. The rate of condensation, ρ, can be evaluated in a mathematically clean way by using the so-called spectral projectors[2]. Based on gluon field configurations generated by the CLS international collaboration, the rate of condensation of the low modes has been computed in QCD with two light flavours[3,4], see figure 1. ρ is clearly different from zero in the chiral limit for Λ = 0.

The smoking gun for the presence of spontaneous symmetry breaking in QCD is the agreement between the chiral-limit value of the rate of condensation at the origin and the slope of $M_\pi^2 F_\pi^2/2$ with respect to the quark mass m^{RGI} in the chiral limit, where M_π and F_π are the mass and the decay constant of the Nambu-Goldstone bosons. The study[3,4] was thus complemented with the computations of m^{RGI}, M_π and F_π.

The results show that the low quark modes do condense in the continuum as expected by the Banks--Casher mechanism, and the rate of condensation agrees with the slope of $M_\pi^2 F_\pi^2/2$ with respect to the quark mass, i.e. the Gell-Mann-Oakes-Renner (GMOR) relation. Indeed, the numerical value obtained for the rate of condensation of the low modes in figure 1 predicts the pion mass dependence seen in figure 2.

This is a numerical proof that the picture of spontaneously broken chiral symmetry in QCD is indeed correct. This has been possible thanks to the numerical resources provided by Fermi.

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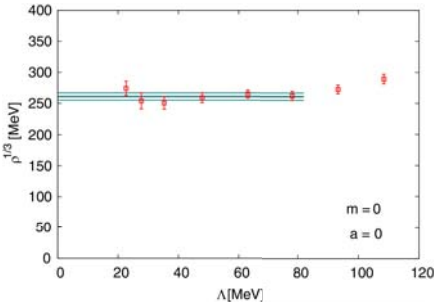
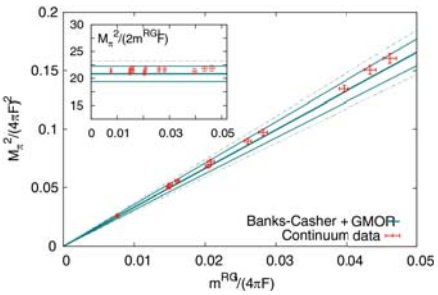


Figure 1
The cubic root of the rate of condensation, $\rho^{1/3}$, of the low modes of the Dirac operator as a function of the mode value Λ. The results are obtained by extrapolating lattice data at finite quark mass and lattice spacing to the continuum and chiral limits.

Figure 2
The pion mass squared versus the quark mass, both normalised to $4\pi F$ which is roughly 1 GeV. The ratio $(M_\pi^2/2m^{RGI}F)^{1/3}$ is the continuum value obtained by extrapolating the lattice data to the continuum limit. The central line is the GMOR contribution to the pion mass squared computed by taking the direct measure of the ratio of condensation of the low modes of the Dirac operator. The upper and lower solid lines show the statistical error and the dotted-dashed ones the total error, the systematic being added in quadrature.



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High-resolution hybrid simulations of the ion-scale spectral break of solar wind turbulence

The solar wind is an exceptional laboratory for plasma astrophysics thanks to spacecraft in-situ observations. One of the best established observational results is the presence of a turbulent cascade over a very large range of scales. A transition between magnetohydrodynamic and kinetic turbulence, characterized by a steepening of the magnetic field spectrum, is observed at scales close to the ion characteristic scales, namely the ion inertial length and the ion Larmor radius. However, observations do not provide a clear evidence on which of the two is associated to this change, nor on which are the physical processes behind it. The project investigated the ion-scale spectral break of solar wind turbulence by performing a large set of 2D high-resolution hybrid simulations, exploring three orders of magnitude in the plasma beta (the ratio of the plasma pressure to the magnetic pressure). Among other things, we recovered the double power-law behavior of the magnetic field spectrum, the ion-scale break and the steepening at sub-ion scales [Figure 1]. The position of the break is related to the ion inertial length for low beta and to the ion Larmor radius for large beta [Figure 1, inset], consistently with solar wind observations. While turbulence develops many current sheets are observed to generate around and between coherent structures of the magnetic field. Once formed, these quickly disrupt due to the onset of fast reconnection. Our analysis suggests that most of the current structures develops at ion scales, indicating that the ion-scale transition seems to be mainly due to the dissipation occurring in reconnecting current sheets.

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Acknowledgments
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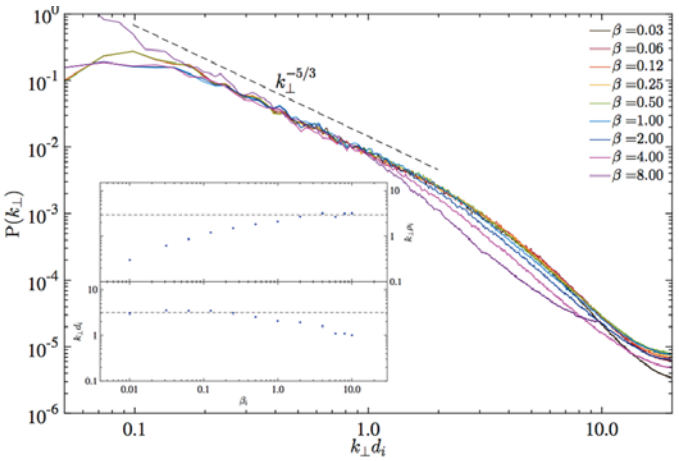

Figure 1
Power spectra of magnetic fluctuations in simulations with different values of the plasma beta, versus the perpendicular wavenumber in units of the ion inertial length.
Inset: Wavectors associated with the spectral break, normalized to the ion Larmor radius (top half) and to the ion inertial length, versus beta.

An Efficient Computational Approach for the Calculation of the Vibrational Density of States

The vibrational density of states of a molecule is the number of vibrational states per unit of energy. This quantity is of paramount importance in molecular and chemical physics. Information about energetics, thermodynamics at equilibrium, as well as molecular spectroscopy can be obtained from the knowledge of the density of states. In general, to calculate the vibrational density of states directly and with high accuracy for large systems is a difficult task. The challenge ahead of us was to include not only anharmonicities but also inter-mode couplings and quantum effects.

An implementation to achieve this goal was already provided by John. R. Barker and collaborators at Michigan State University as part of the MultiWell kinetic modeling program suite. Once the density of states is known, the partition function can be easily derived and it is used for the computation of thermal rate constants for the elementary steps of reaction networks. The original MultiWell code for the evaluation of the vibrational density of states (adensum) is based on a special Monte Carlo procedure, the Wang Landau algorithm. Unfortunately, this code can be applied only to systems of moderate size, due to the large computational overheads needed. For this reason, MultiWell is usually employed to model the kinetics of reactive systems with low number of atoms, which are anyway relevant for atmospheric and combustion chemistry.

The aim of our project has been to extend the range of applicability of the original serial implementation by parallelizing it (with the MPI paradigm), to open up the possibility of kinetic modeling with MultiWell for relevant reactions in organic chemistry. The parallelization strategy we employed is to divide the energy range into windows and set the calculations of the vibrational density of states for each window on a single processor. This strategy is driven by the observation that fewer random sampling events and reduced computational effort is needed for Monte Carlo convergence in a restricted energy range. We have tested the accuracy of our new paradensum code on several molecular systems, including some benchmarks for which an exact evaluation of the vibrational density of states is doable by direct counting. In addition, we have found a significant computational speedup when applying our code to molecules up to 66 vibrational degrees of freedom. Furthermore, our new code can easily handle 150 vibrational degrees of freedom. These features make paradensum a very promising tool for future calculations of thermodynamic properties and thermal rate constants of complex systems.

The outcomes of this project have been published as a research paper[1], presented in June 2016 at the international workshop "Different Routes to Quantum Molecular Dynamics" held at CECAM-HQ, EPFL, Lausanne, Switzerland. The paradensum code is now freely available upon request and it is implemented in the latest 2016 version of MultiWell suite of codes (http://clasp-research.engin.umich.edu/multiwell/index.php). The authors are now official developers of the program suite.

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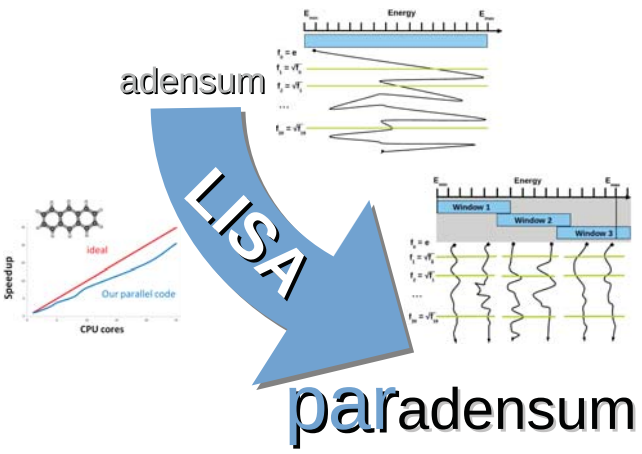

LISA

Two dimensional Silicon-Germanium HEtero-structures for Innovative devices

Among the novel two-dimensional materials, Silicene and Germanene, two honeycomb crystal structures composed of a mono-layer of Si and Ge respectively, are focusing the interest of material scientists because they combine the advantages of the new two-dimensional ultimate-scaled electronics, with their compatibility with industrial processes presently based on Silicon and Germanium. We propose a new type of pseudomorphic planar heterostructures based on ribbons of Silicene and Germanene, which are the two-dimensional analogous of conventional three-dimensional Si/Ge super-lattices and quantum wells.

In spite of the considerable lattice mismatch (~ 4%) between free-standing Silicene and Germanene, our first principles simulations predict that, considering striped two-dimensional lateral hetero-structures made by alternating Silicene and Germanene ribbons of constant width, the Silicene/Germanene junction remains pseudomorphic - i.e. it maintains lattice matched edges - up to a critical ribbon widths that can reach some decades of nanometers. Such critical widths are one order of magnitude larger than the critical thickness measured in three-dimensional pseudomorphic Si/Ge heterostructures, and than the resolution of state-of-the-art lithography, thus enabling the possibility of lithography patterned Silicene/Germanene junctions.

We computed how the strain produced by the pseudomorphic growth modify the crystal structure and electronic bands of the ribbons, providing a mechanism to engineer the Fermi velocity of high mobility carriers within the Dirac cone. Our results pave the way to lithography patterned lateral heterostructures that can constitute the building blocks of the novel two-dimensional electronic devices.

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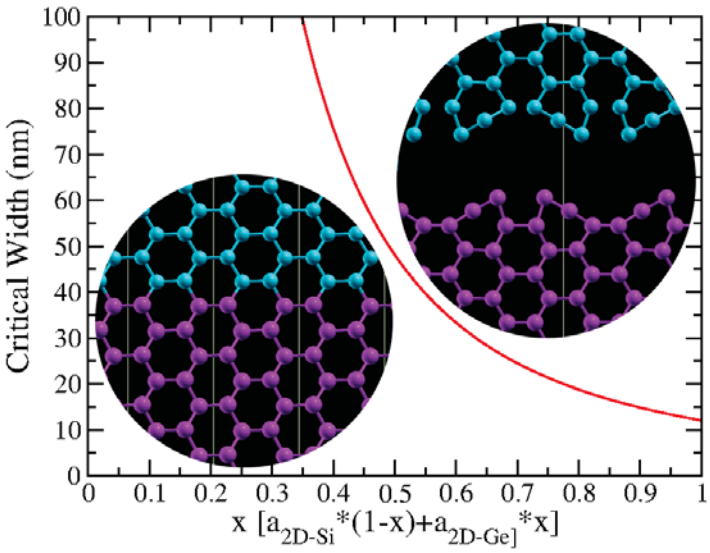

Critical width of Silicene epi-ribbon as a function of lattice parameter of a Germanene seed-ribbon (assumed of macroscopic size) for armchair (red solid line) inter-edge. In the round inserts: top view of the 2D crystal structures used to simulate the armchair 2D pseudomorphic hetero-junction for epi-ribbon width lower than the critical width (left insert) and the surface-edges of the corresponding structures when the epi-ribbon width is grater than the critical width (right insert). $a_{2D\text{-}Si}$ and $a_{2D\text{-}Ge}$ denote the lattice parameter of free-standing Silicene and Germanene, respectively.

Acknowledgments
This project was supported by a LISA program (2-SGHEI).

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ISBN 978-88-86037-35-8