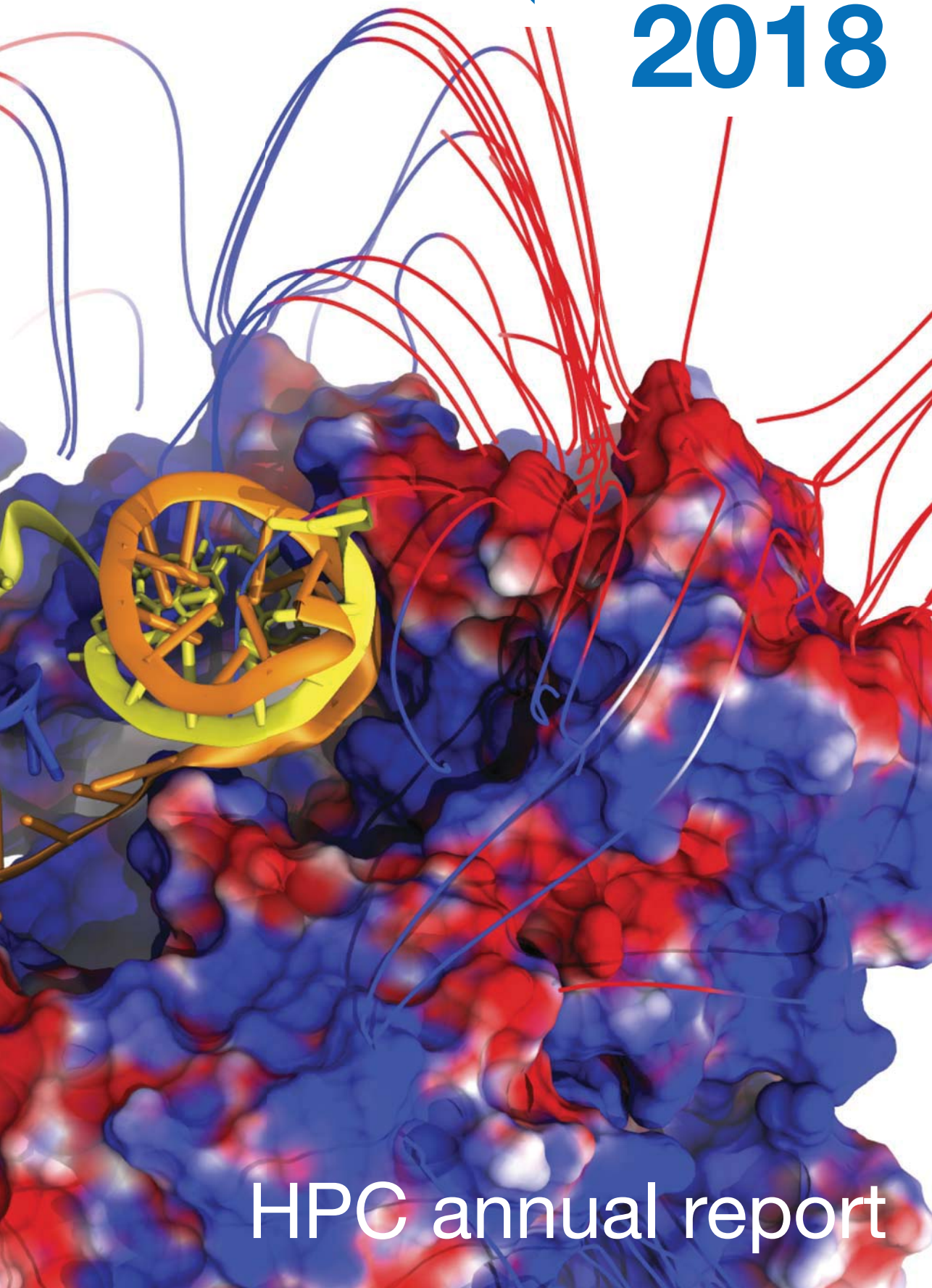
CINECA 2018



HPC annual report

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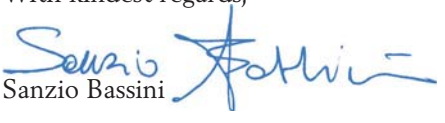
CINECA 2018

HPC annual report

Dear Colleagues,
The annual report of HPC has always represented a milestone and a connection between what has been achieved in the previous year and the objectives for the current one. This is particularly true on this occasion, perhaps more than at any time before.
Over the past year, from the point of view of the objectives achieved, we have obtained very important results in all areas of the Department's activities.
The MARCONI project, key in our supercomputing architecture evolution, reached its final configuration in this period. This was made possible also thanks to joint development actions between Cineca, INFN, SISSA/ICTP, various Universities and the award of a computing service contract for the 2019-2023 period by the Eurofusion community.
Cineca confirmed its commitment to promoting research and development activities as is evident from the many newly funded projects in which Cineca is a primary partner in almost all the domains of the HPC value chain, from HPC Centres of Excellences to new projects in the domain of digital twins, artificial intelligence and HPC technologies. In addition, there have been also new projects funded at the national level in the domain of augmented and virtual reality applied to the digital humanities, cloud computing services and vertical services for specific communities such as that of bioinformatics.
The support for the innovation and the development of the HPC ecosystem around Cineca received a substantial boost in the last year due to the finalization of a project for the creation of a new Science Park (Tecnopolo), designed to host the HPC facilities of the ECMWF, Cineca and INFN. Each one is independently managed and dedicated to specific typologies of services towards the scientific community, but at the same time, there is a synergic vision regarding the promotion of technologies and skills around what it may become an important HPC hub at the world-wide level.
Although this list of brilliant successes achieved in 2018 could be longer, during the last year there was an event that certainly represents a turning point in the HPC ecosystem for Europe and its Member States and that will have an impact on the global HPC race to exascale.
I refer to the creation of the EuroHPC joint venture, already signed so far by 28 European States. This report includes a contribution that describes the general objectives, the mobilization of economic resources, both from the Commission and from the participating countries, and the long-term vision for the development of the European HPC ecosystem as a strategic resource for the European development process and its competitiveness in the global economic scenario.
This represents an example similar as to how the ECMWF data centre was brought to Italy, i.e due to the efforts of the government, national and regional institutions, and the scientific community, united in a collaboration with a precise goal and an ambitious intent.
All this made it possible to develop a project to host in Italy, managed and exploited by Cineca, a pre-exascale class system and a long-term national strategy for HPC that will be consistently developed during 2019 and which will represent the guideline for the next period.
We will be able to discuss all this in the near future.

With kindest regards,



Sanzio Bassini

Director of High Performance Computing Department of Cineca

GENERAL OVERVIEW

EUROPEAN PROJECTS

HPC INFRASTRUCTURE EVOLUTION

SCIENTIFIC OVERVIEW

USERS' PROJECTS

GENERAL OVERVIEW

Cineca HPC is the main center for scientific computing in Italy. We run a large computing infrastructure and make it available to Italian and European researchers, as well as to important Italian companies within a programme for supporting national industrial competitiveness.
Here we present data about usage and users, projects and events and, last but not least, our educational activity in the field of High Performance Computing.

HPC infrastructure

Elda Rossi
Cineca

In year 2018, the main event affecting the HPC infrastructure has been the further enhancement of Marconi.
This Tier-0 system started its life in mid-2016, with the set-up of the first partition (A1) based on Broadwell chips and a computational power of 2PFlops peak. After several upgrades and inclusions, at the beginning of 2018 it was configured in three partitions: A1, made of 720 Broadwell nodes; A3, with 2.306 SkyLakes nodes; and A2, a scale-out partition made of 3.600 many-cores node (KNL), with a total peak performance of about 20PFlops. This system was ranked for the TOP500 list in June 2018 at position no. 18, with a sustained performance (Rmax) of 8.413TFlops.
This configuration has been further enhanced in October 2018, with the upgrade of all A1 nodes to SKL, in order to face the requests of a new agreement with the EUROfusion consortium (see pag. 46).
At the end of 2018, the final configuration of Marconi is the one reported in the table on the right.
This supercomputer takes advantage of the 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 for about 10 PByte net.
This system was ranked for the TOP500 list in Novembre 2018 and reached position no. 19 with a sustained performance (Rmax) of 10.385 TFlops.

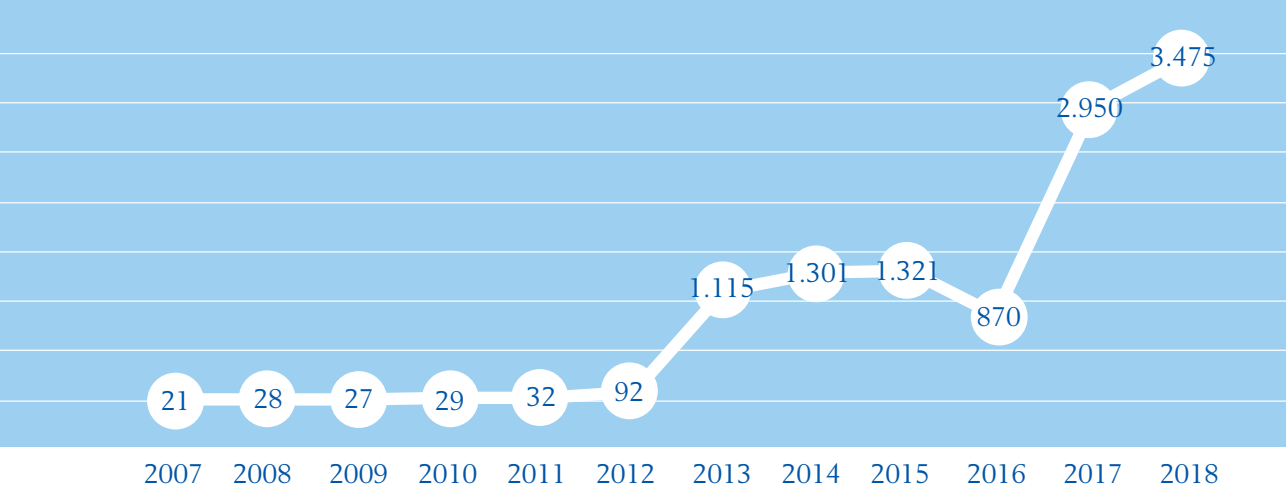
Tier-0

	CPU	Total nodes/ cores	Memory/ node
MARCONI A2 - KNL	Intel Knights Landing 1x Intel Xeon Phi7250 @1.4GHz 68 cores each	3.600 nodes 244.800 cores	96 GB
MARCONI A3 - SKL	Intel SkyLake 2x Intel Xeon 8160 @2.1GHz 24 cores each	3.216 nodes 154.368 cores	192 GB

Tier-1

	CPU	Total nodes/ cores	Memory/ node
GALILEO IBM NextScale Intel QDR (40Gb/s) Infiniband	Intel Broadwell 2 x Xeon E5-2697 @2.1GHz 36 cores each	360 nodes 8.280 cores	128 GB
DAVIDE OpenPower cluster Infiniband EDR (2Gb/s)	2 x Power8+ 4 Tesla P100 SXM2 16 cores each	45 nodes 720 cores	256 GB

As far as the Tier-1 "National" level is concerned, it is actually made of two systems: Galileo and D.A.V.I.D.E.
Galileo, introduced first in 2015, has been reconfigured at the beginning of 2018 with Intel Xeon E5-2697 v4 (Broadwell) nodes, and is available for Italian research community.
D.A.V.I.D.E. (Development of an Added Value Infrastructure Designed in Europe) is based on Power Architecture and coupled with NVIDIA GPUs with NVLink. It is in operation since mid-2017 as the result of a EU funded project and in 2018 it has been made available to general users.

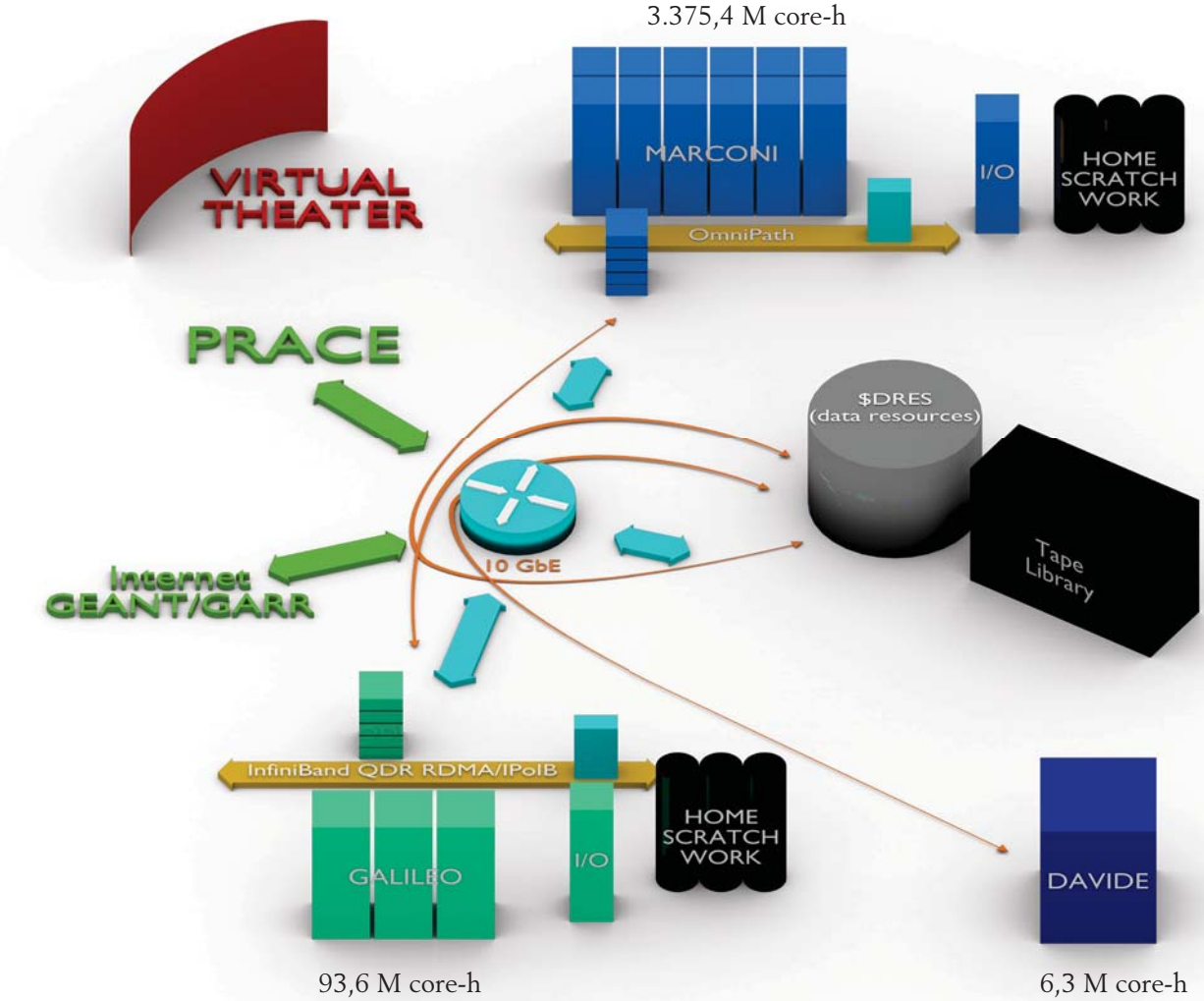


M core-h scientific production.

The computational capacity of these systems is usually expressed in terms of core-h, the number of computing hours that can be exploited for each single core of the system. In the picture below the total annual capacity is reported for each production system, for a grand total of 3,4 billion core-h.

A1: 166,7 M core-h
A2: 2.144,5 M core-h
A3: 1.064,2 M core-h

3.375,4 M core-h



93,6 M core-h

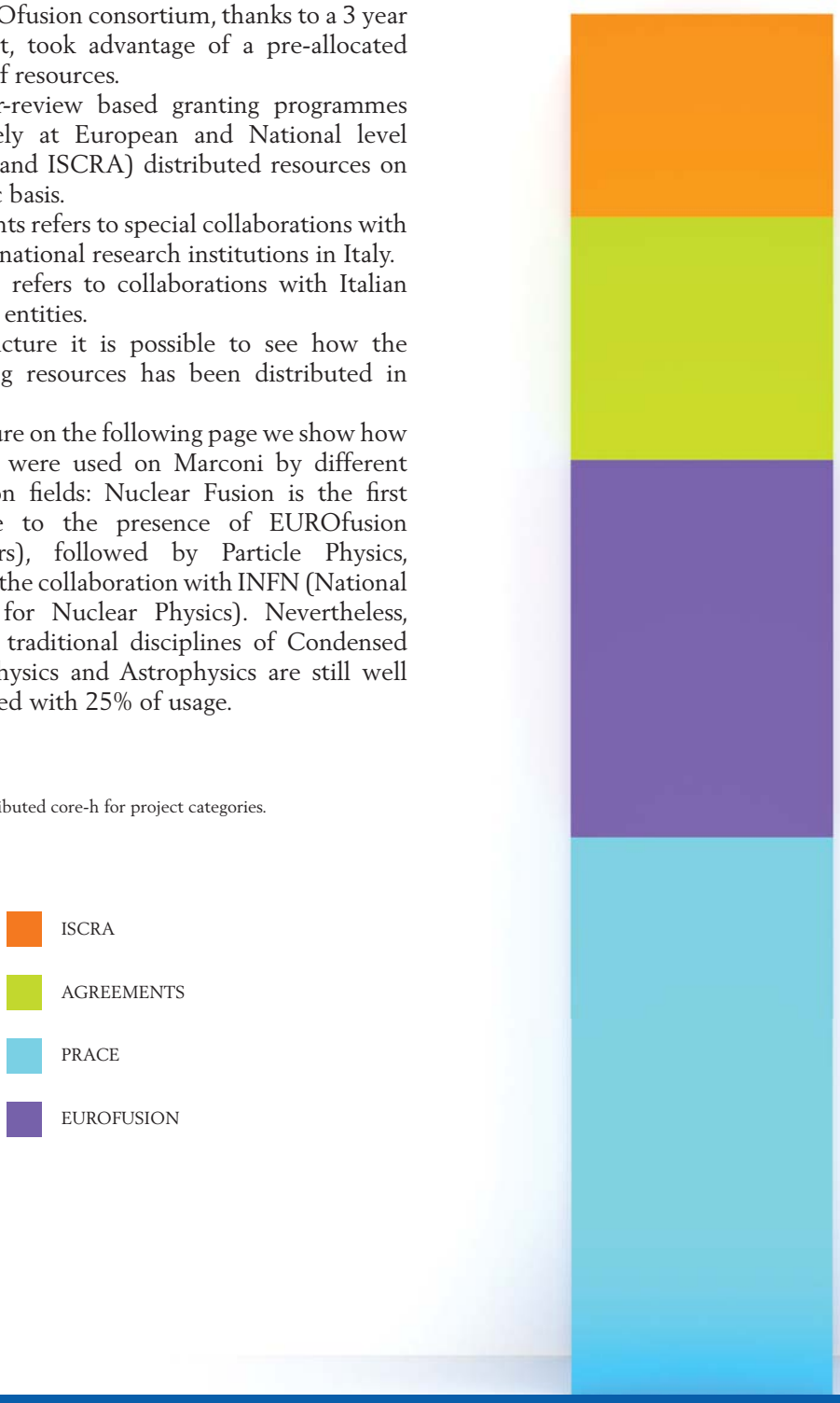
6,3 M core-h

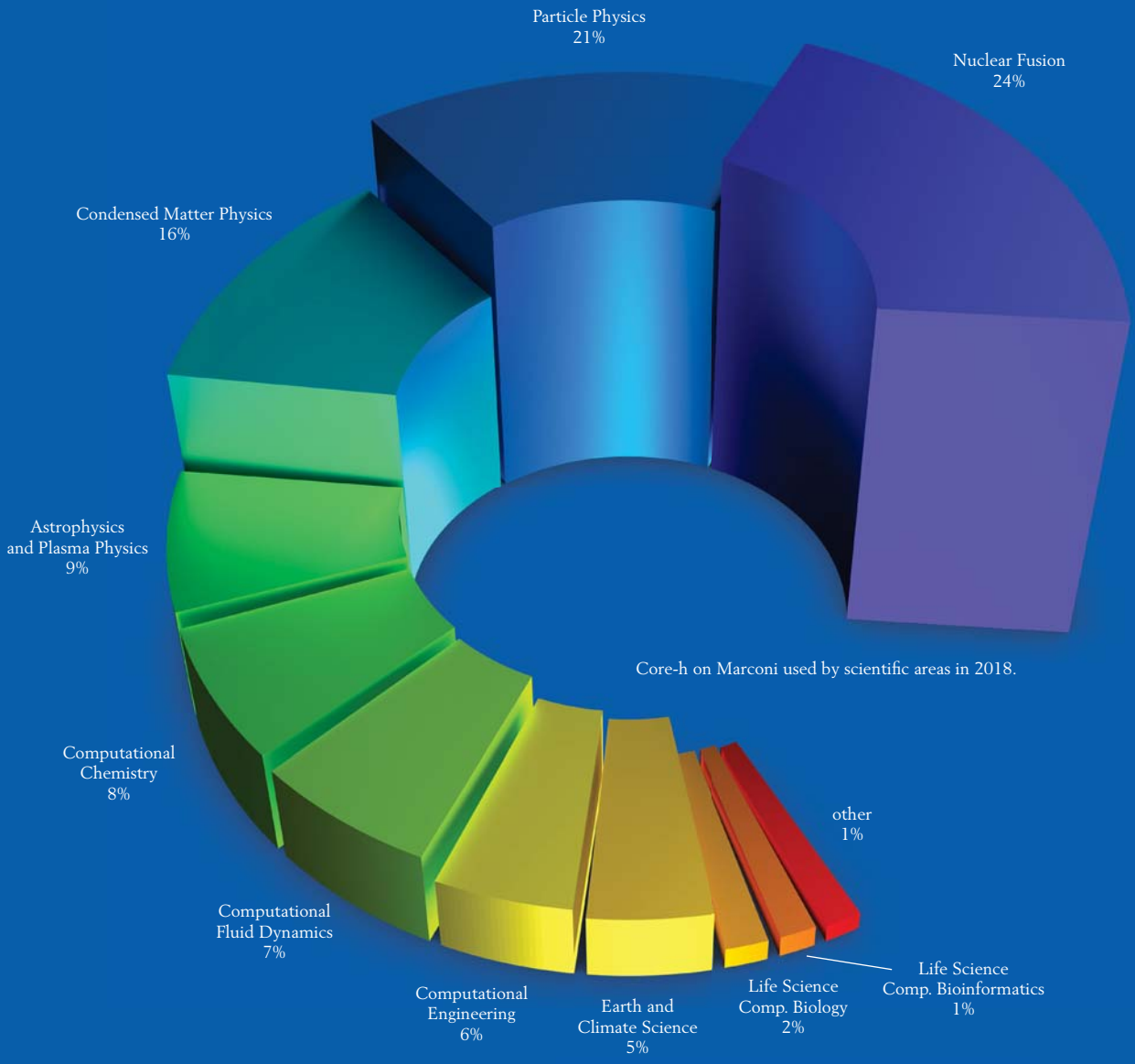
Cineca supercomputing systems and capacity (core-h).

Usage report

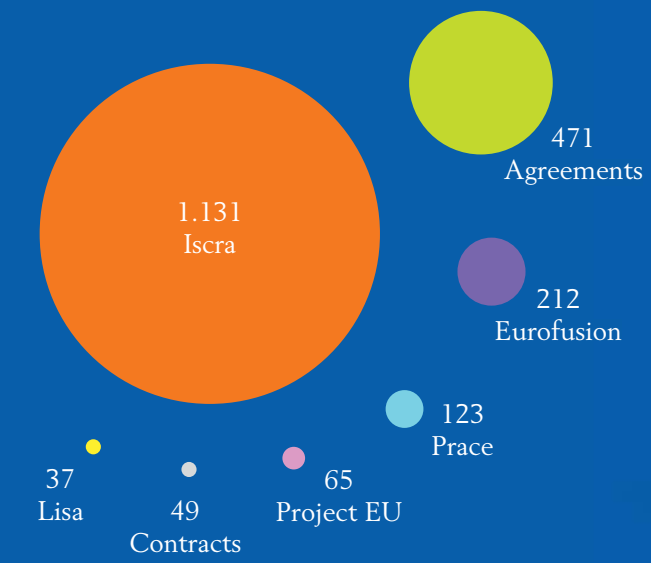
In 2018, as shown here, computing resources have been distributed to Italian and European researchers using different ways.
The EUROfusion consortium, thanks to a 3 year agreement, took advantage of a pre-allocated amount of resources.
Two peer-review based granting programmes respectively at European and National level (PRACE and ISCRA) distributed resources on a periodic basis.
Agreements refers to special collaborations with the main national research institutions in Italy.
Contracts refers to collaborations with Italian industrial entities.
In the picture it is possible to see how the computing resources has been distributed in 2018.
In the figure on the following page we show how resources were used on Marconi by different application fields: Nuclear Fusion is the first one (due to the presence of EUROfusion researchers), followed by Particle Physics, thanks to the collaboration with INFN (National Institute for Nuclear Physics). Nevertheless, the most traditional disciplines of Condensed Matter Physics and Astrophysics are still well represented with 25% of usage.

Marconi distributed core-h for project categories.





Core-h on Marconi used by scientific areas in 2018.



Number of active project during 2018.

494 publications in the 2018

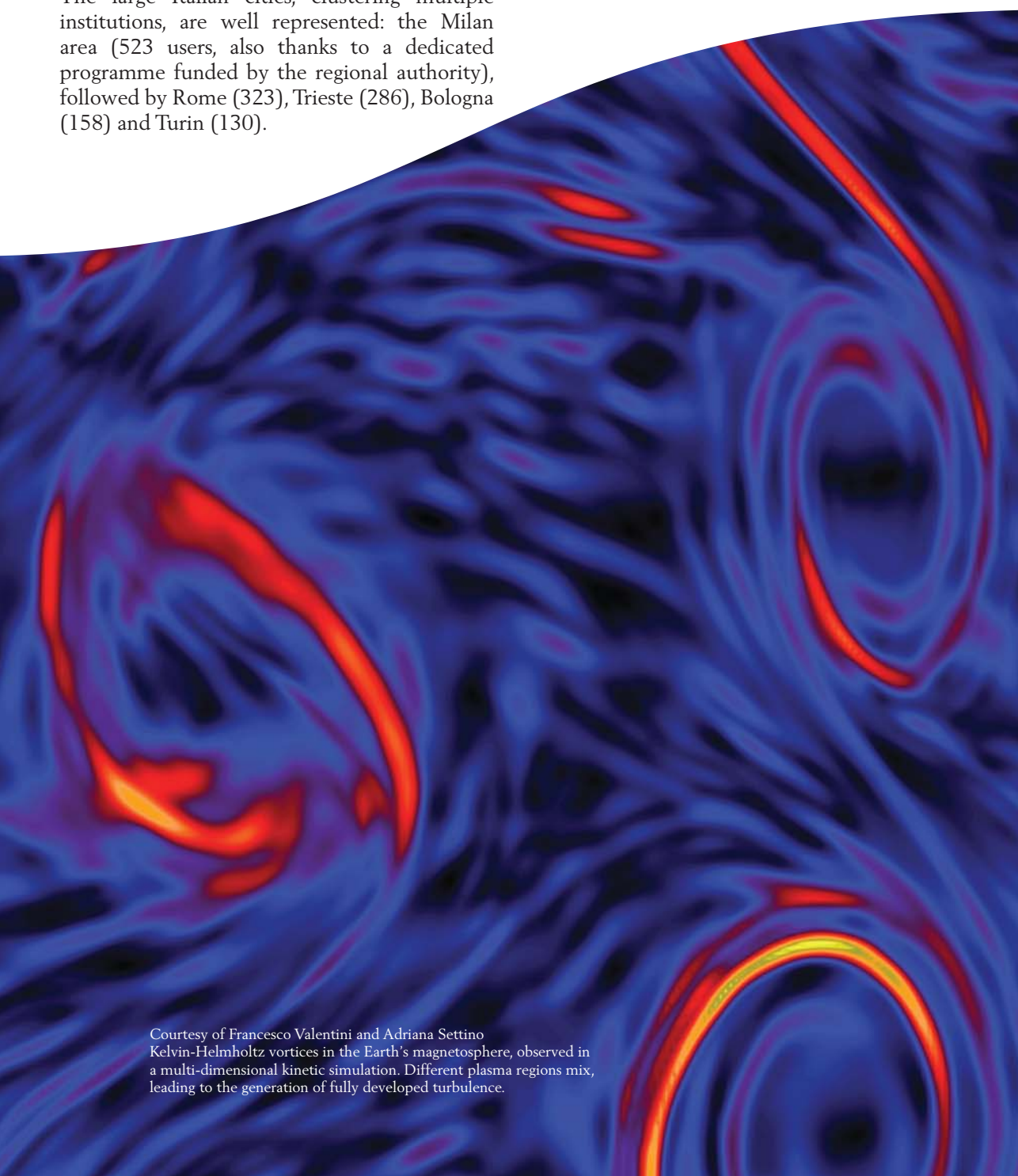
12.886 citations
during the 2018

Information obtained by analyzing the publications using HPC technologies in all the science and engineering fields, citing Cineca.

Users' statistics

During 2018 the active users on our HPC systems were about 3.300. The great majority of the users are males (81%) and working for Italian institutions (66%), mainly Universities or other public research bodies in Italy or abroad.
The large Italian cities, clustering multiple institutions, are well represented: the Milan area (523 users, also thanks to a dedicated programme funded by the regional authority), followed by Rome (323), Trieste (286), Bologna (158) and Turin (130).

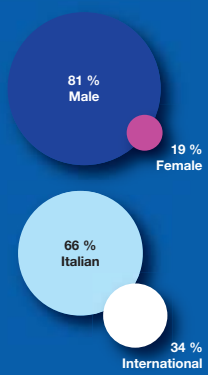
Among the more represented foreign nationalities: Germany and France (thanks to the EUROfusion community), Spain and United Kingdom.



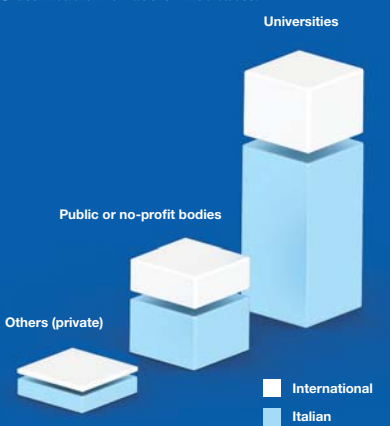
Courtesy of Francesco Valentini and Adriana Settino
Kelvin-Helmholtz vortices in the Earth's magnetosphere, observed in a multi-dimensional kinetic simulation. Different plasma regions mix, leading to the generation of fully developed turbulence.

Cities of the Cineca users' Italian institutes.

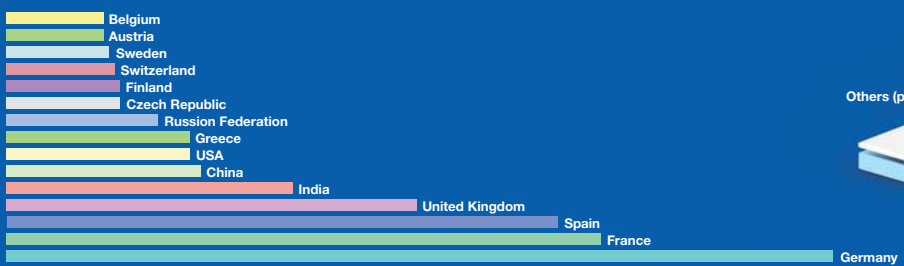
Number of Cineca users by gender and nationality.



Classification of users' institutes.



Nationalities of Cineca users.



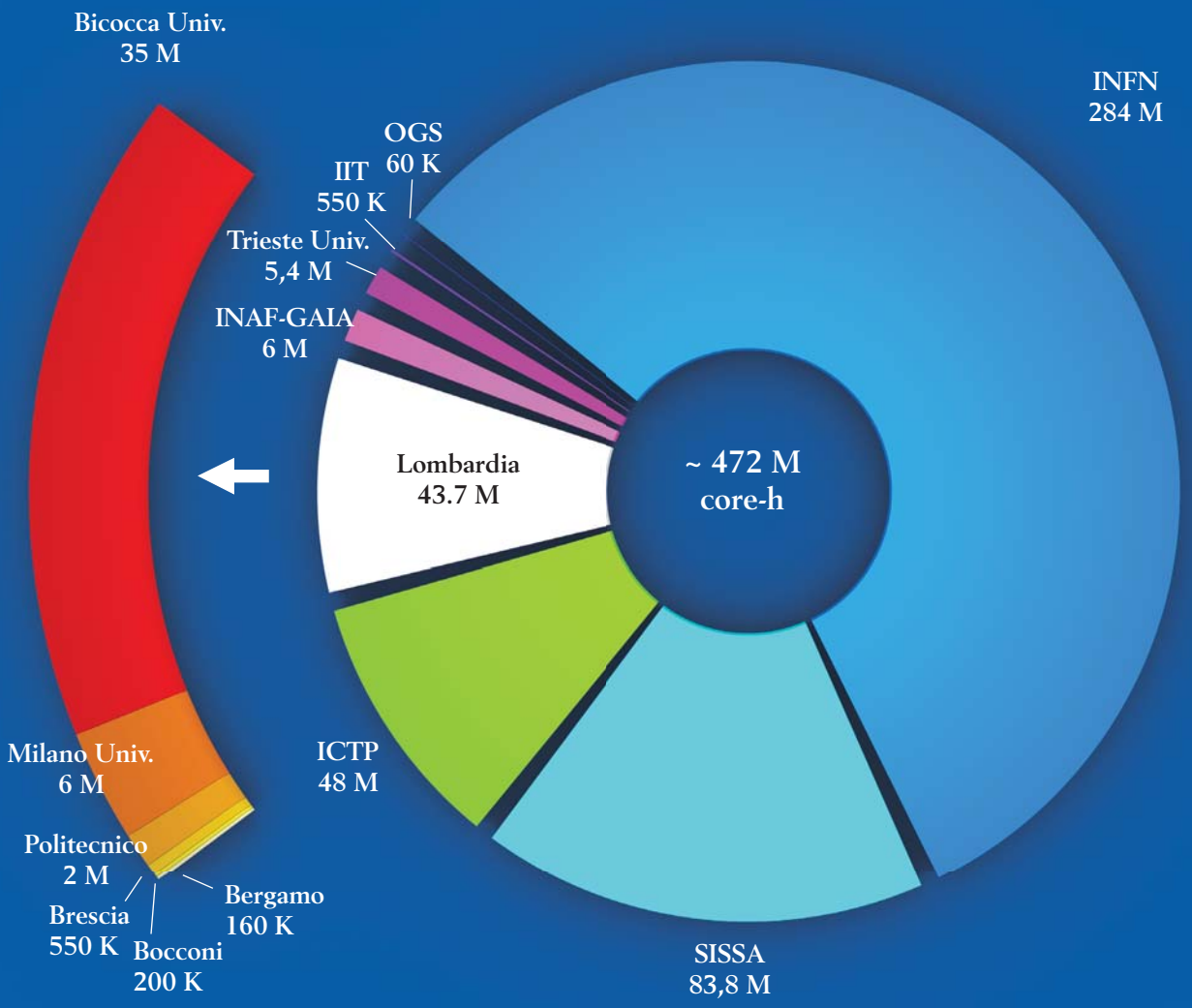
Projects in numbers

Claudio Arlandini and Maurizio Cremonesi
Cineca

Our users get access to Cineca HPC systems by means of projects. Some of them are based on peer-review mechanisms: PRACE is at European level; ISCRA is for national researchers (ISCRA-B are large projects and ISCRA-C small projects); LISA is a programme funded by regione Lombardia for local researchers.
Other projects, defined under the category "Agreements", are collaborations with the main Italian research Institution; "EUROfusion" reports for projects activated within the agreement with the community of nuclear energy; "Contracts" refers to projects with industrial companies in Italy.
The numbers below represent the number of projects active in 2018 for each category:

PRACE: 123
ISCRA - B: 238
ISCRA - C: 893
LISA: 37
AGREEMENTS: 471
EUROFUSION: 212
CONTRACTS: 49

In the picture the allocation numbers in terms of core-h for agreements collaborations are reported.



OTHER AGREEMENTS (~ 8 M CORE-H)

A particular category of projects are in the field of genomics and life-science. They can count on an allocation of about 8 million core-h and take advantage of the collaboration of well-known Italian and European Institutions.

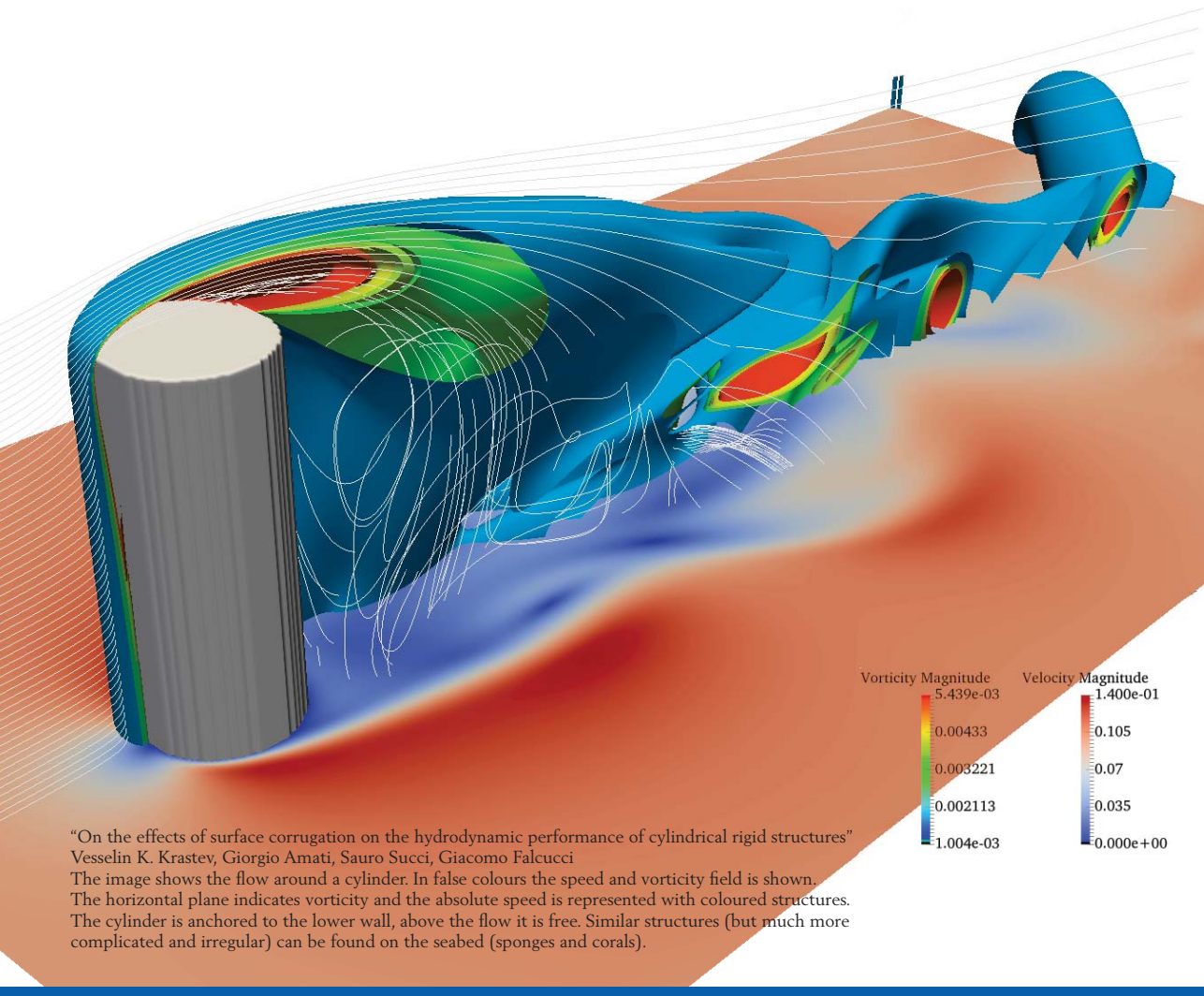
Telethon foundation

ELIXIR (Distributed infrastructure for life-science information)

NIG (Network for Italian Genomes)

INMI Lazzaro Spallanzani IRCCS

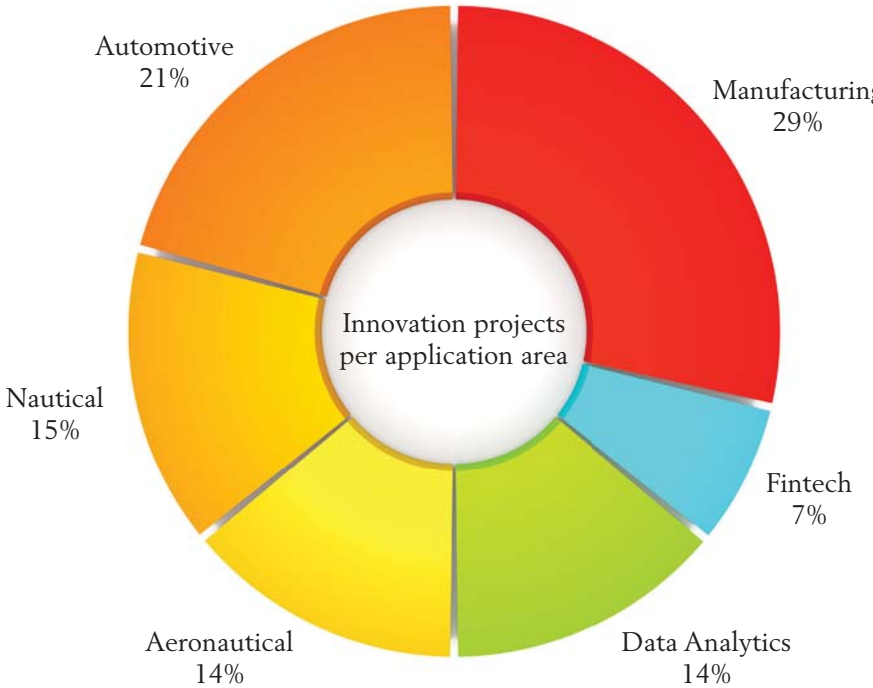
Bambino Gesù



"On the effects of surface corrugation on the hydrodynamic performance of cylindrical rigid structures"
Vesselin K. Krastev, Giorgio Amati, Sauro Succi, Giacomo Falcucci
The image shows the flow around a cylinder. In false colours the speed and vorticity field is shown. The horizontal plane indicates vorticity and the absolute speed is represented with coloured structures. The cylinder is anchored to the lower wall, above the flow it is free. Similar structures (but much more complicated and irregular) can be found on the seabed (sponges and corals).

INDUSTRIAL COMPANIES: INNOVATION PROJECTS

Cineca is involved in several innovation projects, i.e. funded projects primarily consisting of activities directly aiming at producing plans and arrangements or designs for new, altered or improved products, processes or services with the direct involvement of industries, and especially SMEs.



COLLABORATION WITH ENI

For over 15 years, Cineca has been collaborating with Eni (the most important Italian Energy Company) in the set up of the company HPC ecosystem, implementing the most advanced algorithms developed by Eni, developing applications and managing the company HPC systems, initially in Cineca datacenter and, since 2013, in Eni's Green Data Center. On Cineca side, the collaboration involves many people with different skills, able to work in research projects, and in the development and management of HPC applications and systems.
In January 2018, Eni set up its forth generation High Performance Computing System, HPC4, located in the Eni's Green Data Center (GDC). With a peak performance of 18,6 PFlops, the system was ranked 13th in the TOP500 List, emerging as the most powerful HPC system World Wide installed by an industrial company.
HPC4, associated to the other HPC3 system, took the whole Eni's HPC infrastructure to the availability of 22,4 PFlops. This infrastructure provides a strategic support to Eni's digital transformation process along its whole value chain, from exploration to reservoir management to the analysis of all the data generated during the operations.
In 2018 Cineca put HPC4 in production and collaborated with Eni on the evolution and maintenance of HPC applications, as well as on new Eni research projects developing new applications for reservoir simulation, data analysis and interpretation.
In the course of 2018, 40 projects were developed with Eni:

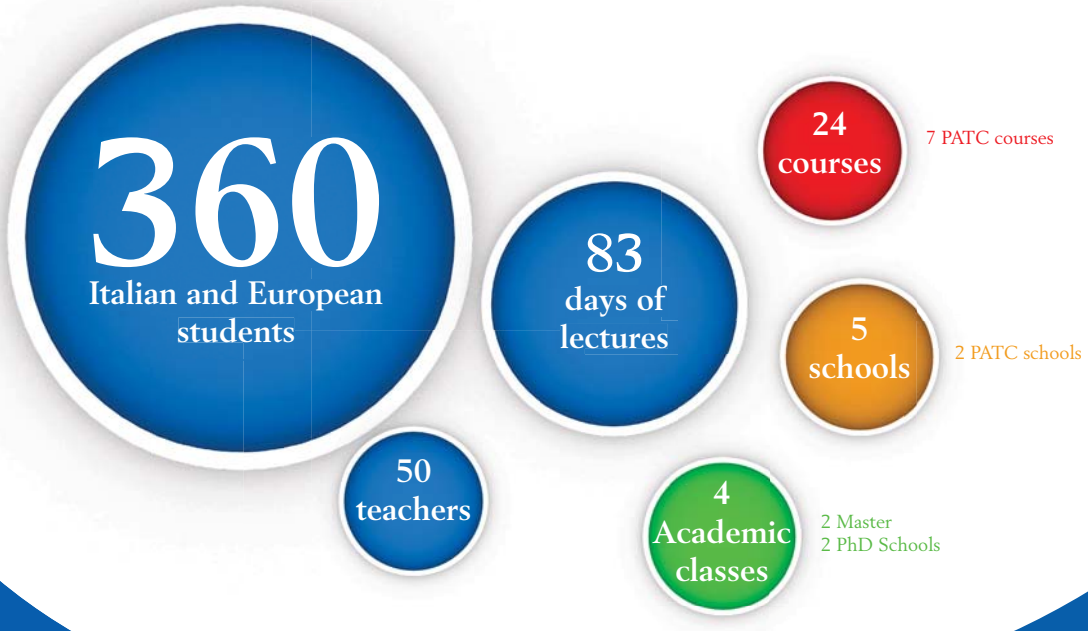
- 5 projects concerned the parallelization, optimization and portability of hybrid codes on different platforms,
- 2 project concerning the evolution of the HPC production environment,
- 13 projects concerned the development and maintenance of production applications,
- 20 projects concerned the development of 5 new applications and 6 new components and new solvers, to be integrated into the production applications.

The collaboration with Eni allowed Cineca staff to face the problems and the typical needs of industrial production, to grow in the understanding of the specific domain and in the ability to work in highly specialized and effective multidisciplinary teams.

Training

Nicola Spallanzani
Cineca

Training has always been a hallmark of the support activities carried on by Cineca for the Italian research community and users. Starting from 2012 it was extended to European researchers, Cineca has being recognised as a PRACE Advance Training Center (PATC) in HPC.
During 2018 we reached quite impressive numbers: 24 classes, distributed across the three sites of the consortium (Bologna, Rome and Milan), 5 schools and 4 workshops. More than 50 people in the department, for a total of 83 days of lessons and highly specialised training. In total, more than 360 Italian and European researchers took advantage of our training program, with high satisfaction levels (8,5/10), as shown by the surveys we regularly administer. Teaching collaborations are also active in academic courses (Masters and Doctorate schools) in several Italian Universities where we are involved in courses about HPC and Big data topics.
Other important initiatives: Summer of HPC (a PRACE initiative offering young students from all over Europe to work with HPC teams); European Researchers Night (Cineca is the coordinator of Society, a European project organising the Night in Bologna and surroundings in 2018-2019); HPC-Europa3 (we are the coordinator of the project offering transnational access to researchers visiting HPC centers).
The Traning activity is regulated by two specific procedures that refers to the ISO standard: ISO 27001:2013 "Information Technology - Security techniques - Information security management system".



Average ratings:
8,5/10

Events

SC18 HPC inspires: Cineca went to Dallas

Daniela Galetti
Cineca

The Supercomputing Conference (SC) is one of the most important events in the HPC community. All sites, vendors and customers that are interested in High Performance Computing and related items meet up in the USA. In 2018 the hosting town was Dallas, Texas.
Supercomputers together with the elaboration of big data by Artificial Intelligence and Deep Learning algorithms daily aim to solve human problems about health care, energy save, chemical and pharmaceutical research, etc.
While SC motto of 2018 was HPC inspires, the human aspect of HPC became humanitarian and the plenary sessions were about big refugees migrations prediction, epidemics prevention on refugees camps and how to quickly reach a medical solution for a very rare disease before it kills a child.
It was really inspiring watching how this gigantic heap of hardware and software thanks to our work can make a world a better place.
People of Cineca team were present not only to improve their professionalism by attending different technical sessions, BoFs and user groups, but also to share their experiences and best practices with the HPC community as one of the 15 largest Supercomputing site.
To better reach this target, as in the last several years, Cineca held a booth at the exhibit, in collaboration with INFN-CNAF.
In 2018 Cineca enriches the communication aspects both in terms of updated information with the last news and results on the booth panels and a new look for the walls of the stand that were rethinked and redesigned by our engineer expert of rendering.
The new panels in fabric enhance the colors, improving the visual impact and made the new structure lighter than the old one, with a better effect on place and an interesting saving of money on shipping expenses. Unlike the previous one, this new stand system is highly modular, so it could be reused in other exhibitions, with different configurations.

...And is already time to think about SC19, because HPC is now! See you in Denver.

SC18
Dallas, TX | hpc inspires.

The European Researchers' Night

Elda Rossi
Cineca

September 28, 2018

The European Researchers' Night is a Europe-wide public event dedicated to science and fun learning. It takes place each year the last Friday of September. Around 30 countries and 300 cities are involved.

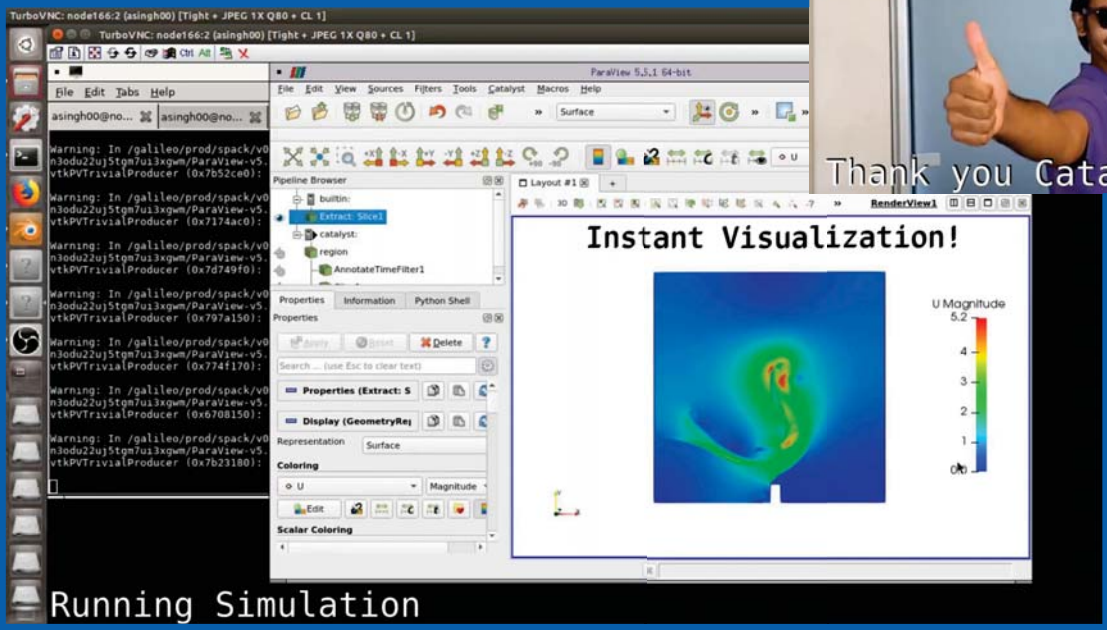
In 2018, Cineca was the principal coordinator of the Night in Bologna, a very successful event that took place in Via Zamboni, together with University of Bologna and all the major local research institutions.
http://nottedeiricercatori-society.eu/

In Rome Cineca participated to a wide collaboration putting together the major research entities and Universities.
https://www.scienzainsieme.it/

Summer of HPC

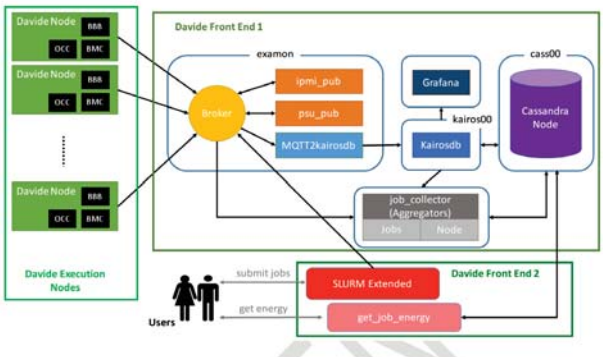
Massimiliano Guarrasi
Cineca

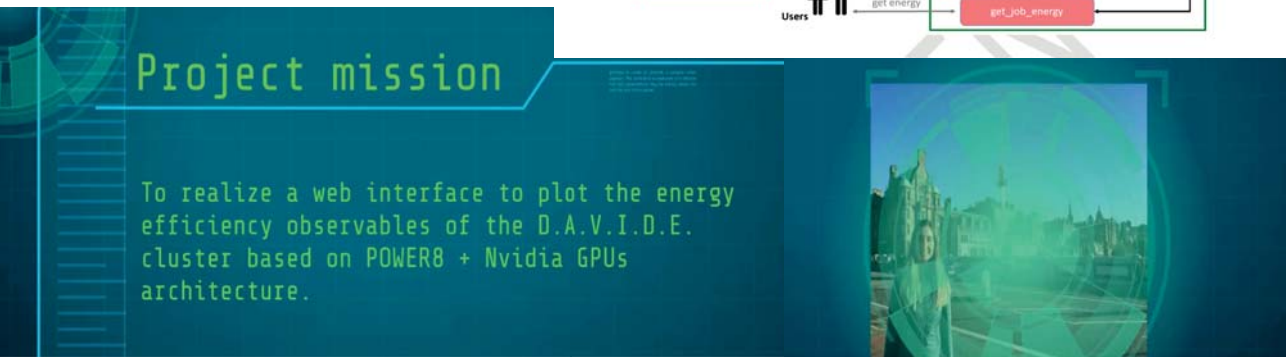
July and August 2018
Summer of HPC is a PRACE (Partnership for Advanced Computing in Europe) programme that offers summer placements at top HPC centers across Europe, in a PRACE partner country. This programme offer to late stage undergraduates and early stage postgraduate students the opportunity to spend two months of the summer at a HPC center. Twenty students go to ten PRACE member centers around Europe, where they worked on PRACE related projects for 2 months during the summer.
https://summerofhpc.prace-ri.eu/



Cineca in 2018 hosted two students:

- Atul Singh, InSitu Visualization with CFD Data using OpenFOAM
- Nazmiye Arslan, Web Visualization and Data Analysis of energy Load of an HPC system





STAFF

In the HPC department of Cineca work about 83 people, distributed into the three premises: 57 in Bologna, 8 in Milan and 18 in Rome.
Several new colleagues were enrolled in 2018: we wish them a very fruitful and interesting job.

Domenico Alberga got a degree in Physics at University of Bari and a PhD in Molecular Simulations. He worked on Molecular Dynamics Simulation of proteins and organic molecules.
In Cineca he is a member of HPC User Support team.

Francesco Cola got a degree in Mathematics at University of Milano-Bicocca. He has a background in calculus of variations and numerical analysis. In Cineca he is working in HPC user support group.

Alessandro Colombo got his master degree in physics at the University of Milan. There, he got also the PhD, which focused on the use of Computational Intelligence for X-Ray Imaging. He is currently part of the group that deals with European projects.

Silvia Gioiosa got a degree in Genomics Biotechnology at Sapienza University of Rome and a PhD in Genetics and Human Biology. She has a background in bioinformatics and big data analysis on HPC infrastructures. She arrived in Cineca in may 2016 with a postdoctoral research fellowship funded by ELIXIR community, a partner of Cineca in the European Roadmap for Bioinformatics project. She was subsequently hired in Cineca in November 2018 with the role of specialistic support to users belonging to Life Science community.

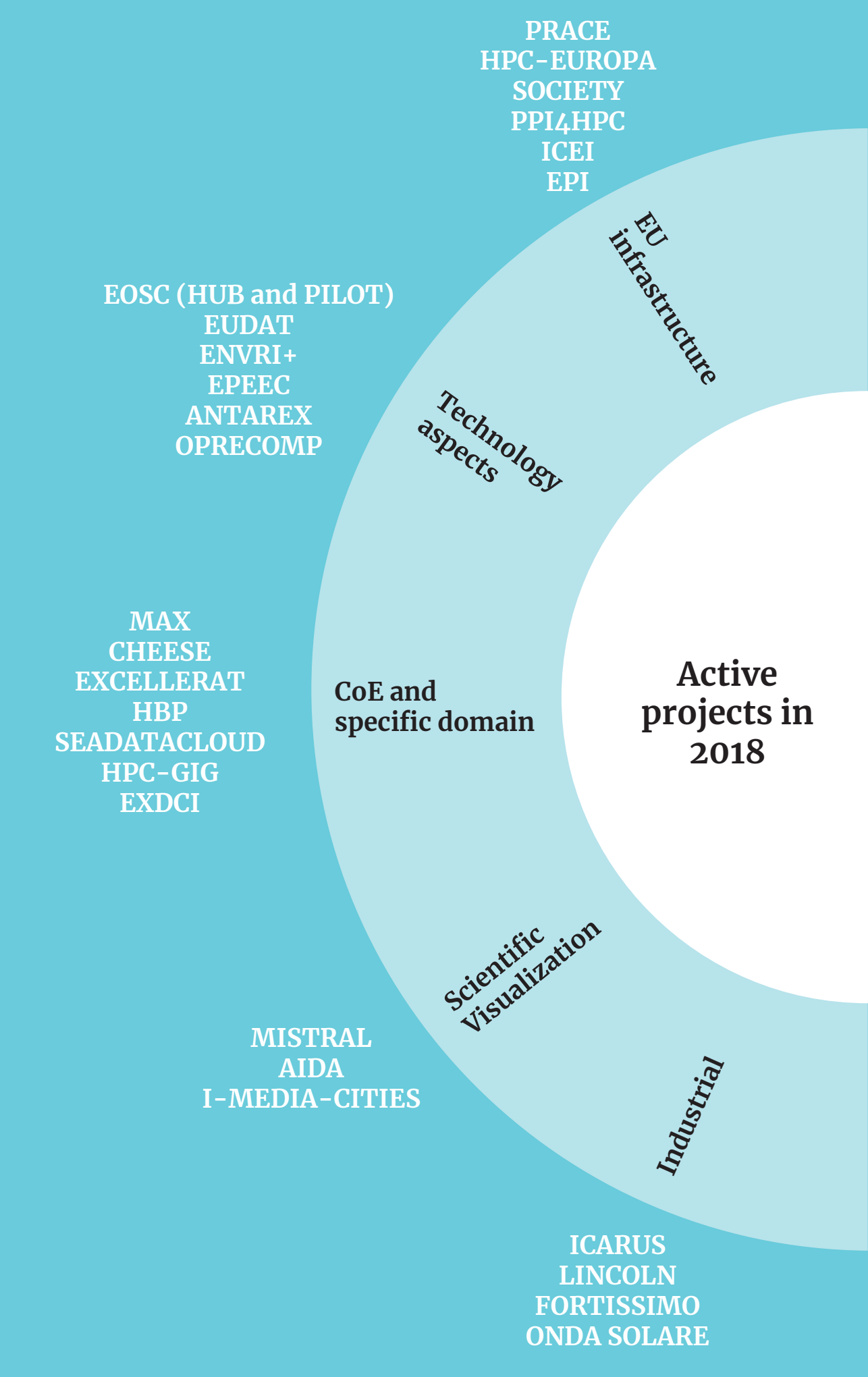
Simone Marocchi got a degree in Chemistry at Sapienza University of Rome and his PhD in Nanosciences and Nanotechnology at University of Modena and Reggio-Emilia. He worked in the Theoretical and Computational Physical Chemistry field on classical and ab-initio methods on nanomagnets and molecules of biological and pharmaceutical interest. In Cineca he is working in HPC service team.

Daniele Ottaviani has got a degree in Applied Mathematics, a second level master degree in Scientific Calculus at University of Rome "Sapienza" and a PhD in Mathematical Models at University of L'Aquila. In Cineca he is working in the field of quantum computing. In March 2019 he participated as a speaker at the European quantum computing conference "Qubits Europe 2019" and at the "OMC" conference in Ravenna. In addition to this task, he also works as a developer in the Eni group.

Fabio Pitari has got a degree and a PhD in Mathematical Engineering at University of L'Aquila. In Cineca he's working in the specialist support for the HPC community. He has a background in the computational chemistry field, in particular on classical and ab initio methods applied on molecular complexes employed in photosynthesis.

Francesco Strappaveccia got his degree in Computer Science at University of Bologna and his Ph.D. in Computer Science at University of Bologna defending the thesis: "Many-core algorithms for Combinatorial Optimization" under the supervision of prof. Vittorio Maniezzo. He spent three years (2015-2018) as Research Fellow at University of Bologna in the H2020 NanoDome project (multi-scale mesoscopic nano-materials modeling and simulation) covering the roles of Work Package leader, HPC developer and technological transfer co-coordinator. Now is working as HPC software developer and GUI developer at Cineca in the ENI support unit.

EUROPEAN PROJECTS


PRACE
HPC-EUROPA
SOCIETY
PPI4HPC
ICEI
EPI
EU infrastructure
EOSC (HUB and PILOT)
EUDAT
ENVRI+
EPEEC
ANTAREX
OPRECOMP
Technology aspects
MAX
CHEESE
EXCELLERAT
HBP
SEADATACLOUD
HPC-GIG
EXDCI
CoE and specific domain
Active projects in 2018
Scientific Visualization
MISTRAL
AIDA
I-MEDIA-CITIES
Industrial
ICARUS
LINCOLN
FORTISSIMO
ONDA SOLARE

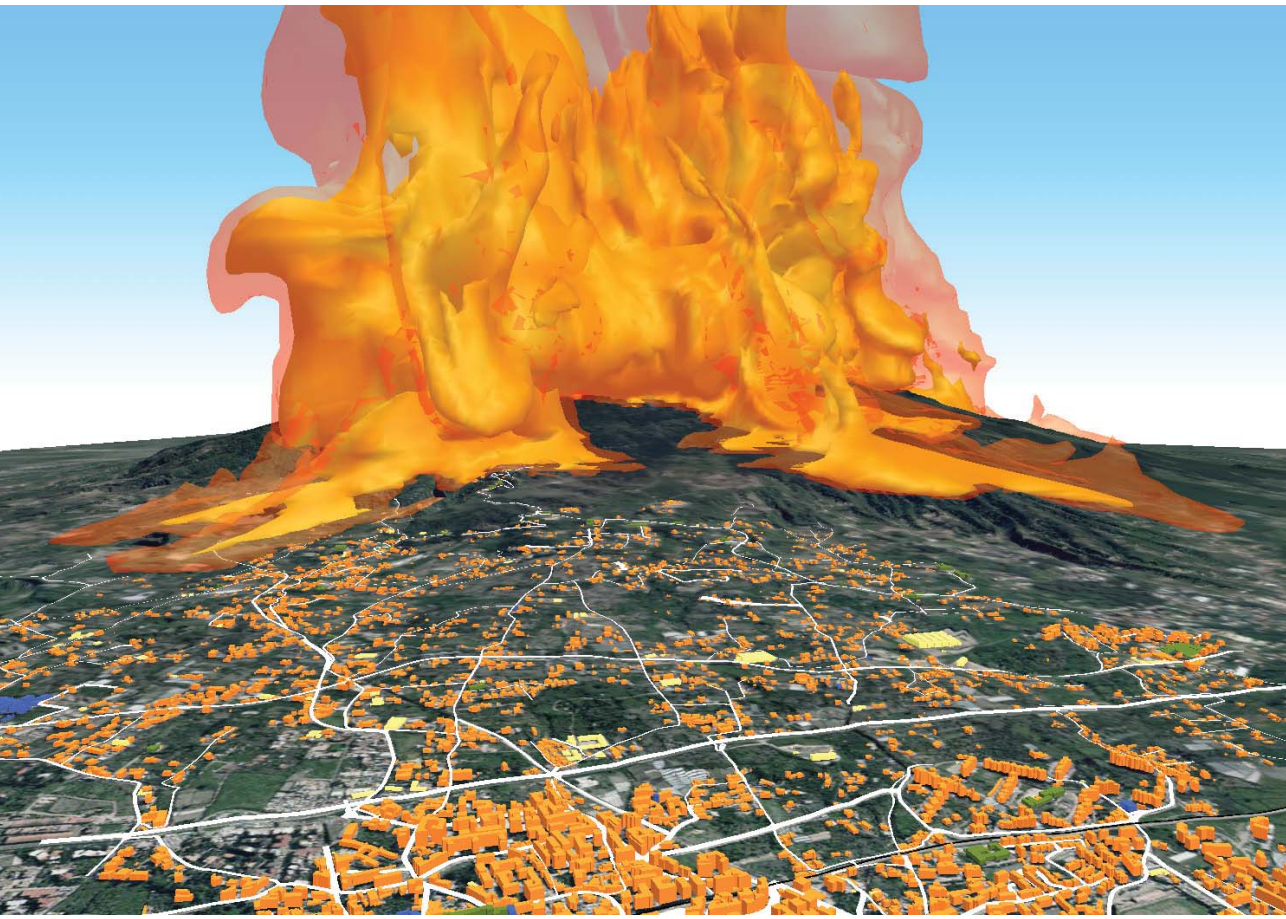
Centers of Excellence

Carlo Cavazzoni, Piero Lanucara, Claudio Arlandini
Cineca

In March 2018 Cineca joined several consortia to propose Center of Excellence on HPC to be funded by the European Commission. At the end of the selection process it was remarkable that three centers supported by Cineca were funded: Cheese, Excellerat and MaX,. Cheese is a project in the domain of solid earth, Excellerat in the domain of engineering and MaX in the domain of material modelling. Of those three MaX was already ongoing thanks to a previous funding program and it was able to be confirmed amid a strong competition.

All three centers started their activities in the second part of 2018 and have the same duration of three years,. The funding for Cineca in the order of 2M€ in total.is significantly Moreover the centers are a strategic asset since they will become part of the EuroHPC initiatives, with the perspective of becoming persistent structures and not only projects.

In the following pages we briefly describe the objectives and the activities of the three centers.



EXPLORIS (Explosive Eruption Risk and Decision Support for EU Populations Threatened by Volcanoes).
The main objective of the project consisted in the quantitative analysis of explosive eruption risk in densely populated EU regions and the evaluation of the likely effectiveness of possible mitigation measures through the development of volcanic risk facilities, such as supercomputer simulation models, vulnerability databases, and probabilistic risk assessment protocols and their application to high-risk European volcanoes.
http://exploris.pi.ingv.it/

CHEESE (CENTER OF EXCELLENCE FOR EXASCALE IN SOLID EARTH)

ChEESE aims to establish a Center of Excellence (CoE) of state-of-the-art codes and related services for upcoming Exascale supercomputing in the Solid Earth domain. ChEESE address extreme computing scientific and societal challenges by harnessing European institutions in charge of operational monitoring networks, Tier-0 supercomputing centers, Academia, hardware developers and third-parties from SMEs, Industry and Public-Governance.
The scientific challenging ambition is to prepare 10 Flagship codes to solve Exascale problems on Computational Seismology (CS), Magnetohydrodynamics (MHD), Physical Volcanology (PV), Tsunamis (T), and Data Analysis and Predictive Techniques, including Machine Learning and Predictive Techniques from monitoring earthquake and volcanic activity:

No.	Code name	Area	Related PD	Partner
1	ExaHyPE	CS	PD4, PD5	TUM
2	Salvus	CS	PD1, PD9	ETH
3	SeisSol	CS	PD1, PD4, PD5	LMU
4	SPECFEM3D	CS	PD1, PD9	CNRS
5	PARODY_PDAF	MHD	PD11	IPGP
6	XSHELLS	MHD	PD11	IPGP
7	ASHEE	PV	PD3, PD6	INGV
8	FALL3D	PV	PD3, PD6, PD12	BSC
9	T-HySEA	T	PD2, PD7, PD8	UMA
10	L-HySEA	T	PD2, PD7	UMA

Cineca is leading the WP2 Work Package, being the place in which the selected codes will be audit and optimized at both intranode and internode level on heterogeneous hardware prototypes for the upcoming Exascale architectures, thereby ensuring commitment with a strong co-design approach.
In parallel with these transversal activities, ChEESE sustent on three vertical pillars.

• To develop pilot demonstrators (PD) for scientific challenging problems requiring Exascale Computing. This includes near real-time seismic simulations and full-wave inversion, ensemble-based volcanic ash dispersal forecasts, faster than real-time tsunami simulations and physics-based hazard assessments for seismics, volcanoes and tsunamis.

• To test selected pilots in an operational environment with the goal to make them available to a broader user community. In collaboration with the European Plate Observing System (EPOS), ChEESE promote and facilitate the integration of HPC services to widen the access to codes and fostering transfer of know-how to Solid Earth user communities.

• To act as a hub to foster HPC across the Solid Earth Community and related stakeholders and to provide specialized training on services and capacity building measures.

EXCELLERAT (THE EUROPEAN CENTER OF EXCELLENCE FOR ENGINEERING APPLICATIONS - EUROPEAN CENTER OF EXCELLENCE)

Engineering applications will be among the first exploiting exascale, not only in academia but also in the industrial sector. In fact, the industrial engineering field is *the* industrial field with the highest exascale potential, thus EXCELLERAT brings together the necessary European expertise to establish a Center of Excellence in Engineering with a broad service portfolio, paving the way for the evolution towards exascale. All within the frame of the European HPC Strategy realization just pushed forward with the activities on the EuroHPC Joint Undertaking.
The scientific excellence of the project consortium will enable evolution, optimization, scaling and porting of applications towards new and disruptive technologies and increase Europe´s competiveness in engineering as such.
To fulfil its mission, EXCELLERAT will base on six carefully chosen reference applications (Nek5000, Alya, AVBP, Fluidity, FEniCS, Flucs), which were selected on their potential to achieve exascale performance and thus to be good candidates to be executed on the Exascale Demonstrators, Pre-Exascale Systems and Exascale Machines.

All the facets of such a center are addressed, from "non-pure-technical" services such as access to knowledge or networking, up to technical services as e.g. Co-Design, Scalability enhancement or Code porting to new (Exa)hardware. Impact is guaranteed by the composition of the consortium, made of key players in HPC, HPDA and Knowledge Transfer, as well as the developers of reference applications. This will ensure a good impact in terms of awareness creation and feedback into the code development itself. The scientific excellence of the EXCELLERAT consortium enables evolution, optimization, scaling and porting of applications towards disruptive technologies and increases Europe´s competiveness in engineering. Within the frame of the project, EXCELLERAT will prove the applicability of the results to other HPC engineering applications besides the six chosen. Thus (but not only for that purpose), the project will extend the recipients of its developments beyond the consortium and use the tool of interest groups to integrate external stakeholders of its value network into its evolution.
The project workplan complements the current activities of the HPC centers involved and fosters the development of next generation engineering applications. Its aim is to support the engineering community at a level that no single HPC provider can.

EXCELLERAT vision is summarised in the following objectives:

• Provide the HPC and engineering community with easy access to relevant services and knowledge

• Provide the HPC and engineering community with access to niche expertise in applications development and offered hardware

• Support the community with targeted training and networking activities

• Integrate users in the evolution of the Center

• Strengthen European competitiveness in the domain of HPC driven engineering through excellent research in the areas of developing, scaling and optimising applications

• Apply innovative engineering solutions enabled by HPC technologies to real world problems

• Facilitate technology transfer from academia to industry in order to enable the latter deliver better, innovative solutions with reduced time to market

The EXCELLERAT project has received funding from the European Union's Horizon 2020 research and innovation programme under the grant agreement No 823691.

MAX (MATERIAL DESIGN AT EXASCALE - EUROPEAN CENTER OF EXCELLENCE)

MaX (Materials design at the eXascale) is a user-driven European Center of Excellence (ECoE) established to support developers and end-users for materials simulations, design and discovery. MaX is focussed at enabling the best use and evolution of HPC technologies by creating an ecosystem of knowledge, capabilities, applications, data workflows, analytic tools and user-oriented services.
MaX is in the domain of material modelling. Materials are crucial to scientific and technological challanges and industrial competitiveness, as well as to tackle key societal issues – from energy and environment, to health care, information and communications, industrial processes and manufacturing, safety and transportation. The increasingly high accuracy and predictive power of computer simulations combined with the raising higher levels of computing power and large amounts of storage capacity of High-Performance Computing (HPC) technologies now enables a paradigm shift in material design and discovery, in which the most complex material behaviour will be addressed by accessible, interdisciplinary, easy-to-use computational experiments.

At the same time, MaX is enabling the Exascale transition in the materials domain by developing advanced programming models, new algorithms, domain-specific libraries, in-memory data management, software/hardware co-design and technology-transfer actions.
MaX is designed and managed to support the needs and the visions of a number of players:
End-users in research and innovation, both in industry and academia, who explore materials discovery and rely on computer experiments.
Domain scientists who develop new methods, algorithms and tools in materials simulations.
Software engineers and vendors who optimise hardware and software performance and usability together with analytical tools for increasingly efficient computer-assisted materials design.
HPC centers and industry who are interested in empowering the most advanced and ambitious solutions and in hardware-software co-design
MaX implementation strategy consists in developing a new application and data ecosystem, and to serve its industrial and academic community through end-user oriented actions. MaX key actions include:
Implementing a Sustainable Programming Platform properly designed quantum engine kernels and low-level domain specific libraries, to facilitating quantum engines advanced functionalities and to share libraries with other communities/domains.
Building a Dynamic Data Framework to manage the automation of high-throughput calculations, automatic data storage, workflows interchange where data provenance, preservation, reproducibility, and reuse are guaranteed.
Promoting the Exascale Transition Enabling Action through the development of novel algorithms, domain-specific libraries, in-memory data management, and software/hardware co-design.
Establishing the User Needs and Solutions Integrating Protocol by aligning the technological offer with leading end-users requirements.
Developing a Catalogue of Services accommodating end-users help-desk and support, communities' integration, industrial outreach, custom development and consulting.
Contributing to the diffusion of material simulations by addressing the skills gap through an integrated offer of Training and Education programs in HPC and computational material science.
MaX will act as a central service hub that will provide project management, coordination and for each of the project members, shifting and reducing cost through sharing resources and effort. To guarantee the quality of the provided services MaX will maintain all toolsets, templates, and documentation of best practices, procedures, and techniques.

MAX core technologies	
codes	Quantum Espresso, Yambo, Fleur, Siesta, BigDFT, CP2K
framework	AiiDA
Domain Specific Libraries	Sirius, FFTXLib, LAXLib

HPC-Europa3: travel, compute and collaborate

Debora Testi
Cineca

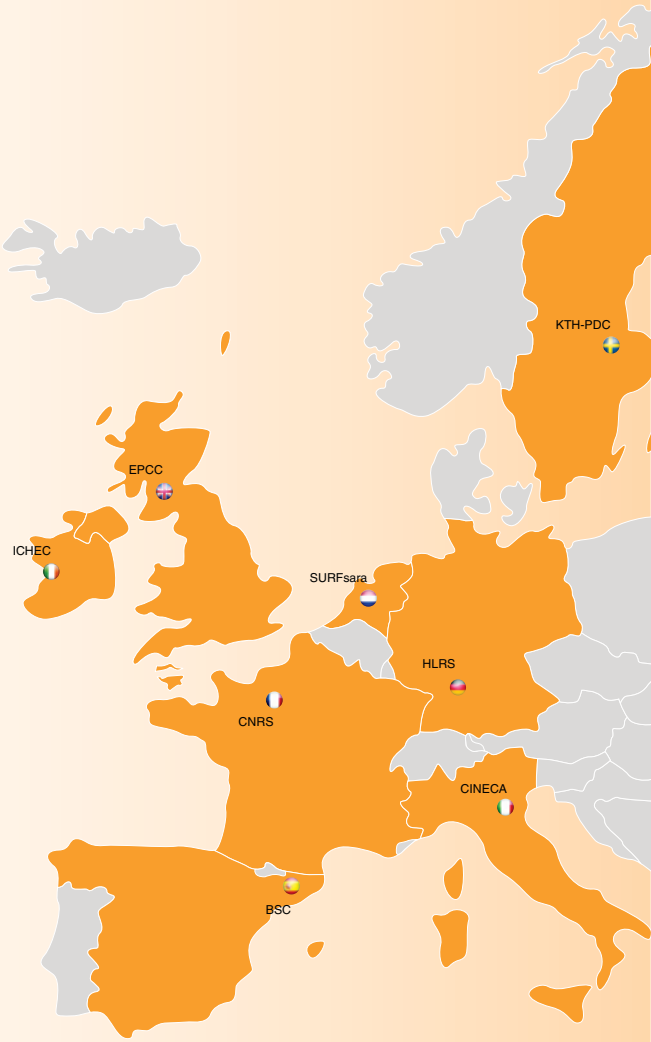
IN A NUTSHELL

HPC-Europa3, coordinated by Cineca, funds international research visits requiring HPC to any of the 9 countries part of the project for 3-13 weeks. HPC-Europa3 reimburses reasonable travel and accommodation costs and provides a small daily allowance. Computing resources and technical support are provided by the local HPC center, while scientific supervision is provided by the host research group. HPC-Europa3 gives additional visibility to the research via social media and the websites of the HPC centers and of course the HPC-Europa3 itself.

HOW TO PARTICIPATE - BE A VISITOR

The programme is open to researchers at any carrier stage working in academia or industry in EU countries or Associated States. The programme continues until 2021 and applications can be submitted any time through an online form. Applications are collected four times a year and are evaluated by the HPC-center, by the host, and by two members of the Scientific User Selection Panel on feasibility, quality of research and suitability for the programme.

http://www.hpc-europa.eu/



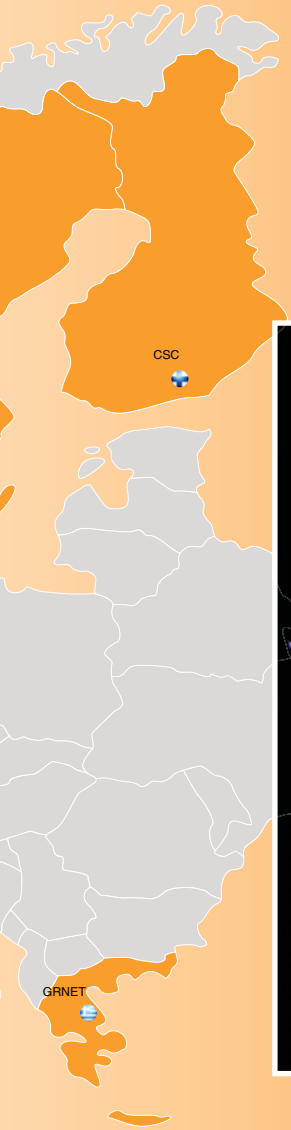
Infrastructure on High Performance Computing
Pan-European Research
HPC Europa3

HOW TO PARTICIPATE - BE A HOST

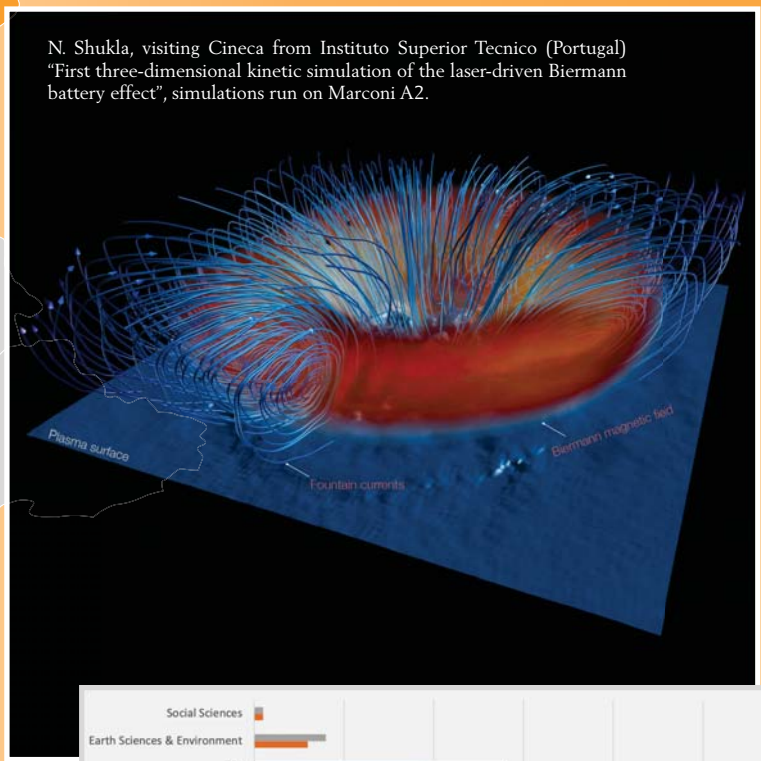
In case you don't want to travel, and you are in one of the countries accepting visitors, you can invite a researcher to your group. You can just agree the research plan with the visitor and sign up as a host on the portal. HPC-Europa3 will take care of the administrative aspects of the visit and you can focus on your research.

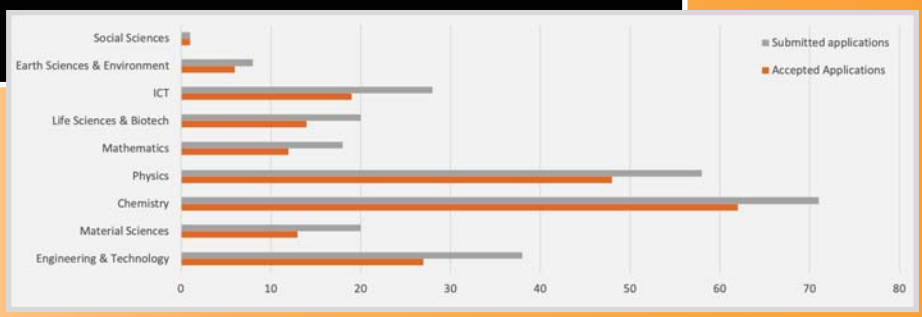
In the first 18 months HPC-Europa3 has supported 204 visits from 48 different countries. Projects are spanning multiple fields of science with most of them concerning either physics or chemistry - fields with a long tradition using computational methods - but also other fields are well represented.

U. Maio, visiting University of Trieste from Leibniz Institut for Astrophysics (Germany), "A simulated galaxy shaped by a dark-matter potential, a stellar bulge and a gaseous disk seen face-on", simulations run on Marconi A2.



N. Shukla, visiting Cineca from Instituto Superior Tecnico (Portugal) "First three-dimensional kinetic simulation of the laser-driven Biermann battery effect", simulations run on Marconi A2.





Participants to the 1st Transnational Access Meeting (TAM), Edinburgh (UK) October 2018.

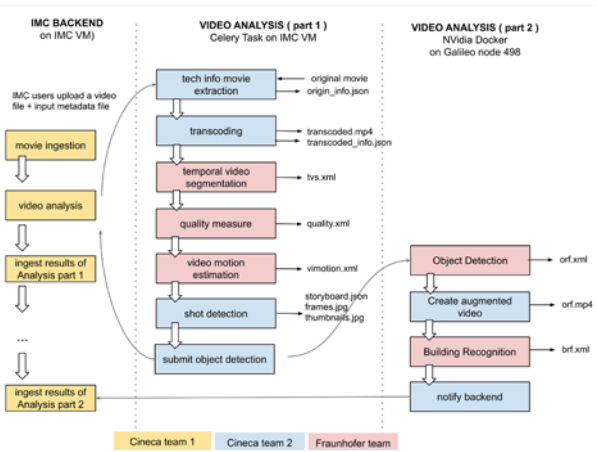
This project has received funding from the European Union's Horizon 2020 Research and Innovation programme under grant agreement No 730897.

I-Media-Cities: an overview

Gabriella Scipione, Antonella Guidazzoli, Maria Chiara Liguori
Cineca

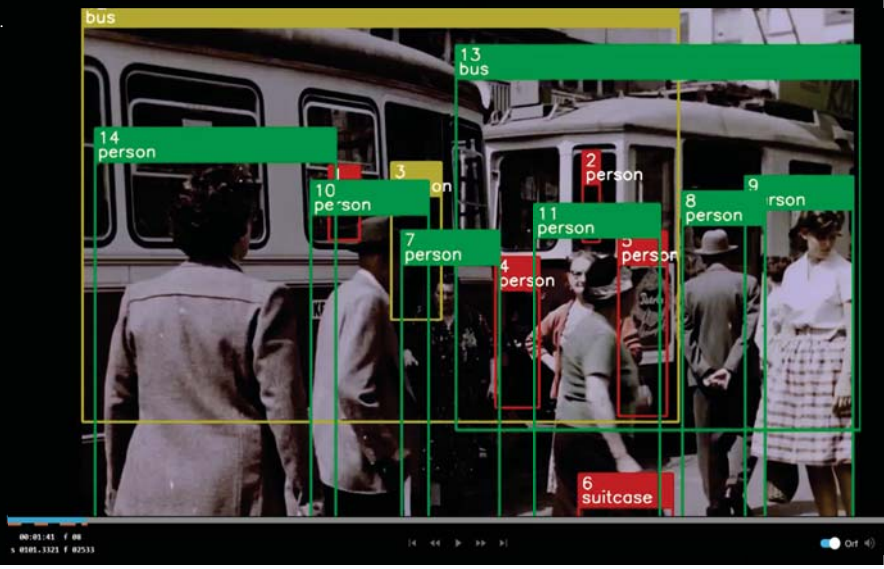
I-Media-Cities (IMC) is a Horizon 2020 EU project that involves 9 audiovisual archives, 5 research institutes, 2 technology providers and a specialist in digital business models (https://imediacities.eu/).
The main goal is sharing automatically and manually enriched audiovisual contents related to the urban environments, encouraging research in the Digital Humanities sector. The project has built an innovative platform through which it is possible to collect, analyze, tag and share the huge amount of audiovisual works from 9 EU film archives - from the late 19th century onwards - describing cities in all aspects, including physical transformation and the social dynamics. The platform involves the creation of different e-environments that will be used by researchers and innovators for new researches and other creative purposes.
The platform receives the contents as videos and images associated to the metadata in XML files provided by the archives. Once the contents and metadata are loaded on to the platform, different algorithms, orchestrated through a pipeline, automatically analyse the videos and extract information and annotate the resource with new metadata, in XML or JSON format, at the frame level or at the level of scene (or shot). The pipeline was conceived in order to treat large amounts of data. The video/image analysis pipeline consists of a set of scripts that runs sequentially and perform data processing for each video imported on the platform. The pipeline manager activates a specific Python thread (also called "worker"), which executes the pipeline scripts. The pipeline produces outcomes as a set of XML-documents containing technical information about the video itself. At the end of the computation the metadata, which had already been provided by the metadata contributing partner, are completed with the information extracted from the pipeline scripts and all this data is stored in the system repository, where it can be queried and retrieved. The I-Media-Cities data model is based on W3C Web Annotation Data Model and is built of three interconnected components for archive metadata, for annotation metadata and for usage related metadata.
All the software components involved in the project system (including AngularJS web portal, Neo4J database and the pipeline scripts) have been installed and deployed on the "Ubuntu Xenial Server" virtual machine hosted the Cineca OpenStack cluster.
The IMC service infrastructure was extended by introducing the possibility of submitting jobs remotely on the HPC nodes. To this extent, the Cineca GALILEO HPC cluster, equipped with GPUs, is instrumented in order to support job submission i.e. using UNICORE middleware, directly from the IMC web portal. Jobs are hence submitted on the HPC cluster using a specific production "Chain" user, which is deputed to submit IMC jobs to the PBS scheduler. This strategy relies upon the adoption of the UNICORE python REST APIs to communicate with the UNICORE framework. Until now 9472 items have been processed, with a computing time of 14,208 hours. The contents, at the moment, have been enriched with a total of 190862 automatic TAG, 52537 manual annotations and 3522 free texts.

IMC Movie Processing Pipeline.

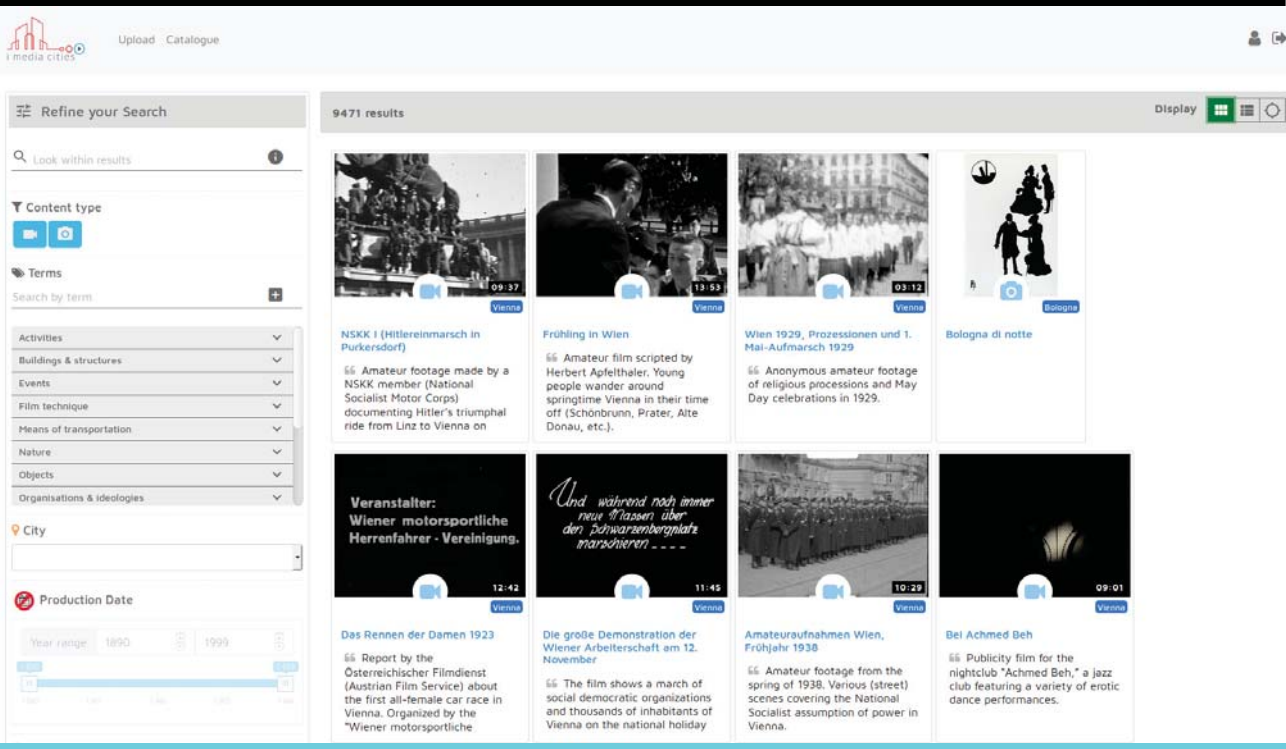


I-Media-Cities Object detection visualisation

I-Media-Cities Object detection visualisation.



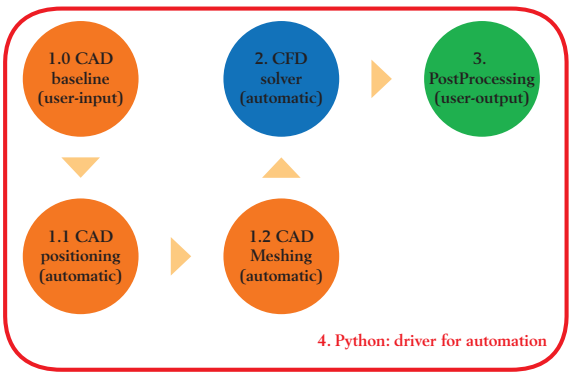
The project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N° 693559.



Onda Solare: HPC technologies to support transportation changes

Raffaele Ponzini and Francesco Salvadore
Cineca

Onda Solare[1] is a wide collaborative project founded by Emilia Romagna Regional Council that aims to develop an integrated path for the conceptual, functional and constructive design of a solar electric vehicle.
The project final target was the construction, in less than two years, of a racing solar car able to participate to the American Solar Challenge. Starting from the design of a new and captivating shape the researchers moved to the 3D final CAD models including the definition of the constructional details for each component, the structural and fluid-dynamic verifications by means of traditional tools, such as wind tunnel tests, and by means of innovative FEM (Finite Element Method) and CFD (Computational Fluid Dynamics) computational codes. The main objective was the ability to proceed with efficiency and speed along the entire design and development process, arriving at a true competition prototype in the scheduled 24 months. The final car, Emilia 4, released in 2018 and able to win the American Solar Challenge, was a solar cruiser with four places, six square meters in plan, less than 300 kg in weight, 120 km/h as peak velocity and 200 km of autonomy.
Cineca is one of the many partners involved in this fascinating innovative manufacturing process. We actively supported the researchers on their day-by-day computational working activities: FEM structural verification and CFD performance evaluation.
In order to support researchers activities related to the computational validation of the structural components of Emilia 4 by means of FEM analyses we developed a simple and intuitive automatic process that enable the final user to submit parallel computations on up to 128 cores using the commercial code Ls-Dyna (Dynamore Inc.[2]) installed on our cluster Galileo. The user can take advantage of automatic process by means of textual user interface (TUI) written in Python programming language that requires only few input parameters to work and takes care of all the hidden technical details to enable parallel job submission, monitoring and data retrieving information by means of automatic mailing.
In a very similar way, we also implemented a fully automatic version of the CFD workflow, necessary for external aerodynamics performances evaluation, based on open source technologies (OpenFOAM[3]).



Automatic CFD workflow.

Starting in April 2016, the Onda Solare project was able to deliver in less than two years Emilia 4, a solar racing cruiser able to participate to the American Solar Challenge and win. We supported researcher's activities by means of effective automatic CFD and FEM workflows that enabled the exploitation of the parallel HPC architectures necessary to perform all the analysis in the scheduled time.

References
[1] Onda Solare web site: http://ondasolare.com/
[2] Ls-Dyna web site: http://www.lstc.com/products/ls-dyna
[3] OpenFOAM web site: https://openfoam.org/

Emilia 4: the final solar car presented in 2018 at the Museo Ferrari in Maranello.

Onda Solare®

Example of fluid dynamics results output at 80 km/h.

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I.I.S. A. Ferrari

2018
American Solar Challenge

Emilia 4 won the category "Multi Occupant Vehicle" and awards for Best Battery Pack Design and Best Mechanical System Design.

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EMILIA-ROMAGNA
2014/2020

UNIONE EUROPEA
Fondo europeo di sviluppo regionale

RegioneEmilia-Romagna

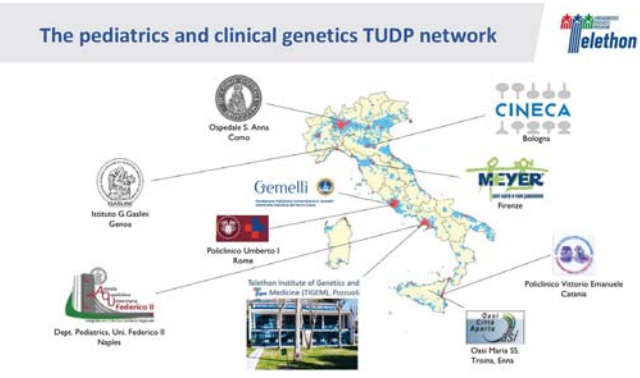
The Telethon Undiagnosed Diseases Program

Giorgio Casari and Raffaele Castello
Telethon Institute of Genetics and Medicine, Naples, Italy

The Telethon Undiagnosed Diseases Program (TUDP) is about solving "undiagnosable" rare and complex genetic diseases. In order to set up such an ambitious program, the Board has started working more than one year before the official start date in 2016.
The program was designed with the aim to find the molecular defect in complex and severe pediatric disorders with the highest chance of represent previously unrecognized genetic conditions using a Next Generation Sequencing (NGS)-based approach.

In few years NGS has shown its tremendous potential for solving undiagnosed genetic conditions. Whole Exome Sequencing (WES) or Whole Genome Sequencing (WGS) approaches have therefore received widespread recognition as universal tests for most Mendelian conditions. As a cheaper alternative to WGS, WES has proved to be an excellent and cost-effective solution with a consistent number of advantages including a higher throughput on coding sequences that favor the disease-genes identification.

Now the clinical network consists of 12 pediatric hubs, strategically located in North, Center and South of Italy (Figure below).
This means that each year the project manages hundreds of patients and relatives data, generating a big amount of genetic data.



Such a huge amount of data needs an uncommon computational capacity that no one of the Centers involved can provide. For this reason and foreseeing this need, Fondazione Telethon and Cineca established an agreement before the start of the project by which Cineca provide Fondazione Telethon with the computational power and storage capacity needed to manage this huge amount of data. Fondazione Telethon, on its side, helps Cineca in creating a repository of genetic data that would increase Cineca knowledge in ambitious genomic projects.
TUDP Bioinformatic Team developed a pipeline, "VarGenius", that executes cohort-level DNA-seq variant calling and annotation and allows to manage the resulting data through a PostgreSQL database.

VarGenius provides a database to store the output of the variant calling analysis (calling quality statistics, variant annotations, internal allelic variant frequencies) and sample informations (personal data, genotypes, phenotypes). VarGenius can also perform the "joint analysis" of hundreds of samples with a single command, thus drastically reducing the time for the configuration and execution of the analyses.
VarGenius has been tested on a Cineca parallel computing cluster of 52 machines with 120GB of RAM each one. Under this configuration, a 50M whole exome sequencing (WES) analysis for a family was executed in about 7 hours (using a trio or quartet did not affect the execution time); a joint analysis of 30 WES in about 24 hours and the parallel analysis of 34 single samples from a 1M panel in about 2 hours. This represent a huge step forward in the analysis of genomic data, thus creating the possibility to analyze cases in a faster and more effective manner, that Telethon would have not been able to do without the collaboration with Cineca.

ICARUS

Giorgio Pedrazzi
Cineca

The European ICARUS project aims to create a new value chain for the aviation sector, based on data sharing and collaboration between operators. The new value created, shared and exchanged enables the renewal of existing processes and the creation of new services and opens the way to new business models. It is therefore a matter of integrating and exploiting data flows from different sources, such as airlines, airports, service providers and local authorities, using the technologies of Big Data, Data Analytics, Deep Learning, Semantic Enrichment and Blockchain.
ICARUS addresses barriers to the adoption of Big Data in the aviation industry (e.g., data fragmentation, data sourcing, ownership and truthfulness, and licensing of use). All this is achieved through the creation of a platform that allows, in a reliable and scientific way, the exploration, care, integration and analysis of the original data and derived data.
The applications developed thanks to ICARUS can bring benefits not only in the aviation sector but also, among others, in tourism, health, safety, land transport and retail sectors. In particular, four demonstration scenarios are developed during the project:

- Management of ground services,
- Analysis of aircraft routes to optimise fuel consumption and reduce pollution,
- Prediction of epidemics with more accurate and realistic models,
- Passenger experience before and after the flight.

Cineca provides to ICARUS the High-Performance Computing and Data Analytics infrastructure for data storage and analysis, it collaborates in the design of the platform and it defines the project's Evaluation Framework.

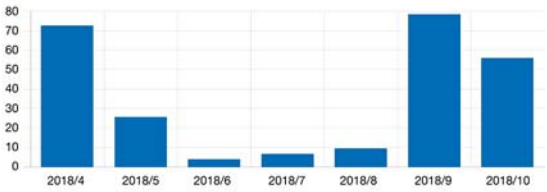
LincoSim: a web application for naval design

Raffaele Ponzini and Francesco Salvadore
Cineca

LincoSim is an innovative web application developed within the European LINCOLN project devised to support the design of planing hulls through the use of computational methods. Since April 2018 the service opened to project partners and today supports three different user groups.

In this report we present the usage experience and statistics of an innovative web application dedicated to support the design process of planing hulls. The web application, called LincoSim[1], was developed as part of the LINCOLN project funded by the European Union[2]. The Web user interface includes highly interactive 2D and 3D WebGL visualizations to prepare, verify, submit and analyze CFD numerical simulations through the user's insertion of the hull geometry and the set of a few physical parameters. The CFD calculation engine uses several standard OpenFOAM solvers[3].

The two main challenges of LincoSim are usability for target users who, as naval designers, are not necessarily CFD experts, and the robustness of the platform itself. From the point of view of strength, it is necessary to consider the quality of all the software used to compose the platform as a whole and the hardware of the virtual machines that host the Web services and the HPC clusters connected to them to carry out the number crunching processes.



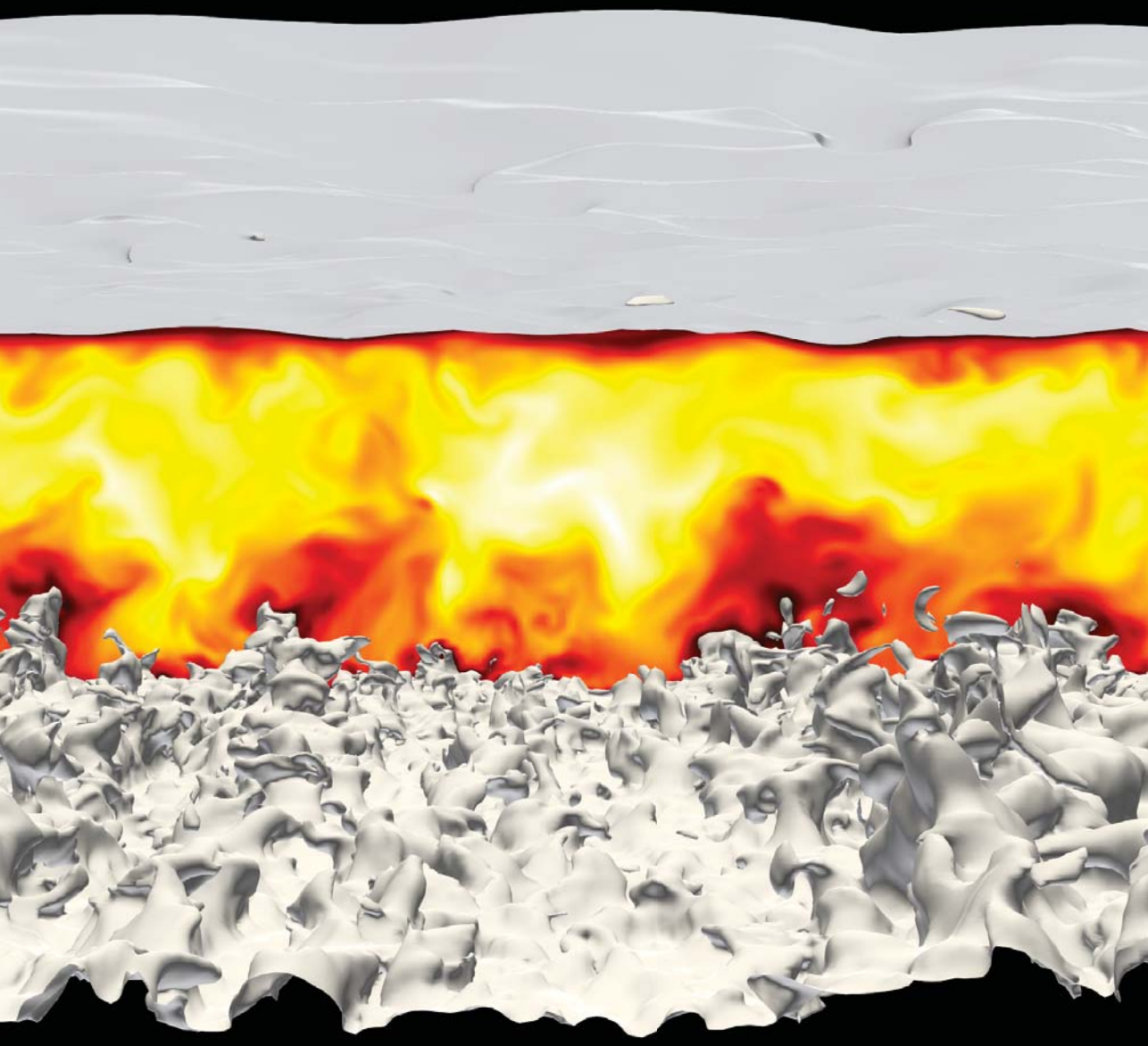
Trend of use of the platform in terms of the number of simulations performed per month.

Starting from April 2018, the LincoSim web application was opened to three groups of industrial partners involved in the LINCOLN project to support the process of designing innovative vessels through automatic CFD analysis. The web service had an up-time of over 99% and hundreds of simulations were made by non-expert users in a few months with reduced failure rates (<6%).

References
[1] LincoSim web access (only for registered users): https://lincosim.cineca.it/login
[2] LINCOLN project web site: http://www.lincolnproject.eu/
[3] OpenFOAM web site: https://openfoam.org/

Types of hull studied.

Courtesy of Alfredo Soldati, Francesco Zonta and Alessio Roccon
Turbulence structures in a viscosity stratified turbulent channel flow, at the top wall, turbulence is largely modulated while, by opposite, at the bottom wall a strong turbulence activity is found.
Results are obtained from Direct Numerical Simulation (DNS) of turbulence coupled with a Phase Field Method (PFM) to describe the interfacial phenomena.



HPC INFRASTRUCTURE EVOLUTION

Cineca is always involved in giving high level computational systems according to its mission for supporting both research and industrial community. Thanks to many industrial and European collaborations new opportunities are growing up.

The evolution in the short term

Carlo Cavazzoni and Elda Rossi
Cineca

SHORT MEDIUM TERM EVOLUTION OF THE HPC INFRASTRUCTURE

In a short term period, let's say in the course of next year, we mainly foresee small changes on the actual infrastructure components.
The major upgrades are expected only in early 2020, with the substitution of our main Tier-0 system (Marconi-A2) with a new scale-out system, suited for extreme parallelism. This is the objective of a European Initiative (PPI4 HPC - Public Procurement of Innovative Solutions for HPC) and it is bringing to Cineca a system of about 30PFlops, five time more powerful than the actual system.
At the same time, another call for tender is open (ICEI - Interactive Computing e-Infrastructure), for the procurement of an interactive system to be made available to the community of the "Human Brain Project" a flagship project in the field of neuroscience and brain-related medicine.
In the short-term, the main change, expected in the first quarter 2019, is the reconfiguration of the Galileo system. The 360 nodes of the actual cluster should increase to over 1.000 nodes, featuring also a more efficient internal network and a larger storage area. This new powerful cluster will be a useful platform for our national users with small to medium parallelism requirement, as well as for Industrial partners interested in a powerful and reliable tool able to boost public and private research competition.
Moreover, not less important, we expect a significant improvement in the infrastructure that hosts the Cloud service for HPC applications. The new system should be into production mid-2019, made of 200 Intel Broadwell nodes configured with ad-hoc solutions for an efficient delivery of the service.

THE ECP PROJECT: THE US ROAD FOR HPC

The Exascale Computing Project (ECP) is focused on accelerating the delivery of a capable exascale computing ecosystem that delivers 50 times more computational science and data analytic application power than possible with DOE HPC systems such as Titan (ORNL) and Sequoia (LLNL). With the goal to launch a US exascale ecosystem by 2021, the ECP will have profound effects on the American people and the world.
The ECP is a collaborative effort of two U.S. Department of Energy organizations - the Office of Science (DOE-SC) and the National Nuclear Security Administration (NNSA).
ECP is chartered with accelerating delivery of a capable exascale computing ecosystem to provide breakthrough modeling and simulation solutions to address the most critical challenges in scientific discovery, energy assurance, economic competitiveness, and national security.
This role goes far beyond the limited scope of a physical computing system. ECP's work encompasses the development of an entire exascale ecosystem: applications, system software, hardware technologies and architectures, along with critical workforce development.

THE EPI PROJECT: THE EU ANSWER

It has been a long time since Europe has had indigenous suppliers of the core components that go into high performance computing systems. The European Union is big enough and rich enough to change that and so its member nations are funding an effort, called the European Processor Initiative, to create a homegrown processor that will be the basis of future exascale machines and that could eventually trickle down into other commercial systems.
The EPI consortium gets together 23 partners from ten European Countries. It gathers experts from the HPC research community, the major supercomputing centers, and the computing and silicon industry as well as the potential scientific and industrial users.
Through a co-design approach, it will design and develop the first European HPC Systems on Chip and accelerators. Both elements will be implemented and validated in a prototype system that will become the basis for a full Exascale machine based on European technology.

The goal is to have an exascale system by 2023, which is an ambitious goal, particularly since they are looking to do it with the semi-new (at least for HPC) ARM processor.
One of the major advantages of ARM is its potential in co-design. This is a fashionable term for customizing a component to better match specific needs, like adding new HPC application friendly instructions to speed up processing. This is something that the EPI is definitely looking to exploit.

Projected Exascale System Dates and Investment levels
Information taken from Hyperion Research 2018.
Related Links: https://eurohpc-ju.europa.eu/

US

- When: 2022-2023
- ES Vendors: U.S.
- Processors: U.S.
- Initiatives: DOE ECI
- Cost: $600M per system (for early system)
- $1 to $2 billion a year in R&D (around $10 billion over 7 years)
- Plans are to purchases multiple exascale systems each year

CHINA

- When: 2021-2022
- ES Vendors: Chinese.
- Processors: Chinese + U.S.
- Initiatives: 5 YEAR PLAN
- Cost: $350-$500M per system
- Over $1 billion a year in R&D (at least $10 billion over 7 years)
- Investments by both governments & vendors
- Plans are to purchases multiple exascale systems each year
- Investing in 3 pre-exascale systems starting in late 2018

EU

- When: 2023-2024
- Pre-ES: 2020-2022 ($125M)
- Vendors: US and then European
- Processors: x86, ARM&RISC-V
- Initiatives: EuroHPC, EPI, ETP4HPC
- Cost: Over $300M per system
- About 5-6 billion euros in total (around $1 billion a year)
- EU: 486M euros, Member States: 486M euros, Private sector: 422M euros
- Investments in multiple exascale and pre-exascale systems
- Large EU CPU funding

JAPAN

- When: ~2022
- Vendors: Japanese
- Processors: Japanese ARM
- Cost: $800M-$1B, this includes both 1 system and R&I costs
- Planned investment of over $1 billion* (over 5 years) for both the R&D and purchase of 1 exascale system
- To be followed by a number of smaller systems ~$100M to $150M each

Europe's and Italy's journey to exascale

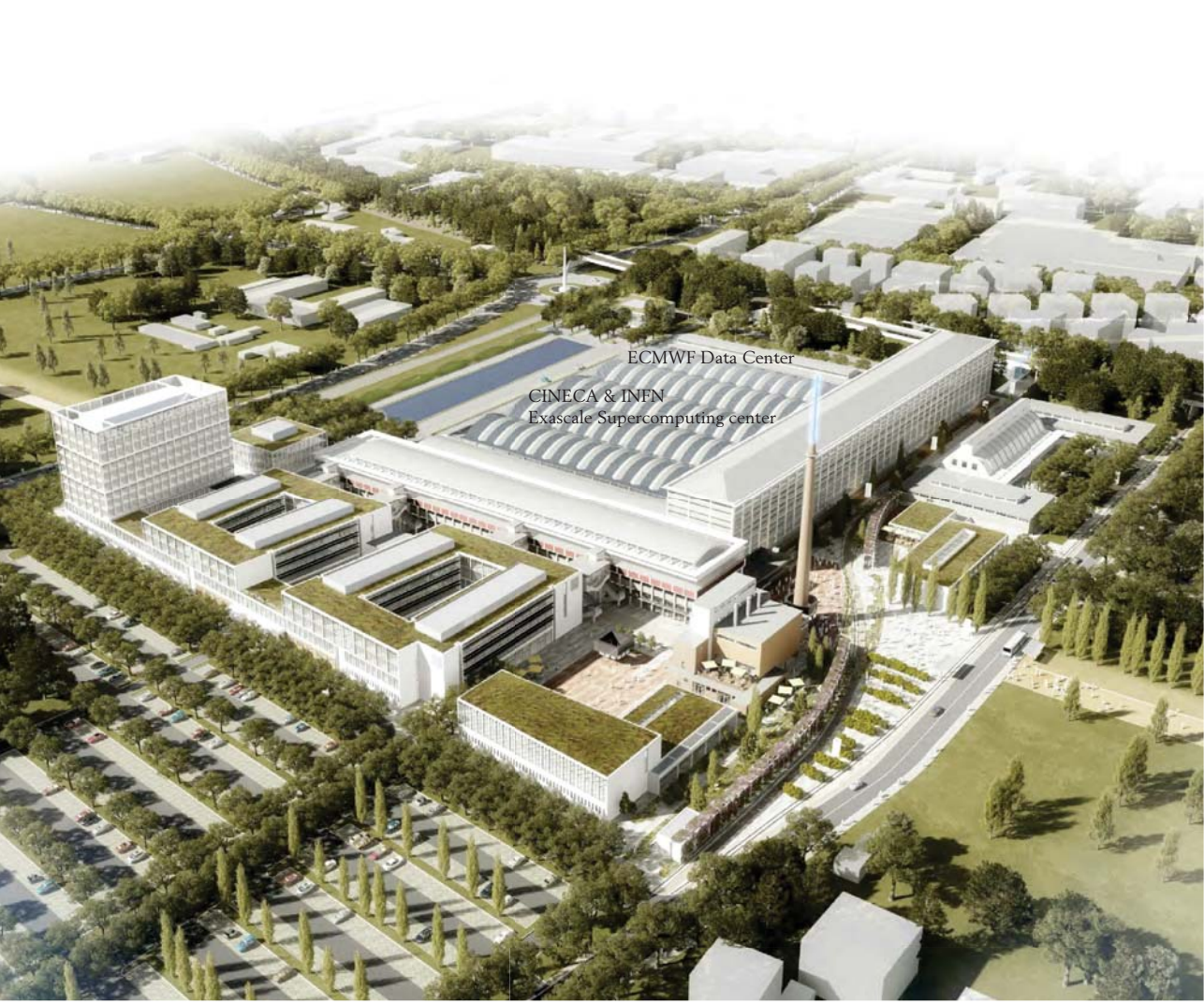
Gabriella Scipione
Cineca

High Performance Computing have become a fundamental tool for scientific discovery in all the scientific domains, facing challenges arising from science, industry and public decision-making. It extends and irrigates fields from different domains: fundamental physics, climate research, biology, life sciences and health, materials sciences. More recently also social sciences and humanities, self-driving cars and financial trading, have benefit from HPC, as well as public decision making support in case of natural risk events.
To face these complex challenges it is more and more necessary to relay on the synergy of advanced algorithms, large size data, and next generation computing technologies as exascale supercomputers.
Great strides have been made by US, China and Japan in these frontiers. As far as Europe is concerned, the computing resources and data available today for European scientists and industry are no longer sufficient to compete on equal terms with the other big players. This is why Europe has recently decided to invest toward a European Exascale computing infrastructures, i.e. capable of achieving performance of the order of the ExaFlops (10^{18} floating point operations).
This initiative, taking place from 2019 to 2026, is implemented through the EuroHPC Joint Undertaking (JU), a legal and funding entity whose aim is to pool European resources to develop and make operational a top-of-the-range exascale supercomputing infrastructure based on competitive European technology.
The European Union, the European Technology Platform for High Performance Computing (ETP4HPC), the Big Data Value Association (BDVA) and 27 European countries, are all participating to the EuroHPC JU, Italy being one of the first that signed the declaration.
The EuroHPC JU will operate through procurements and open calls, with the aim to:

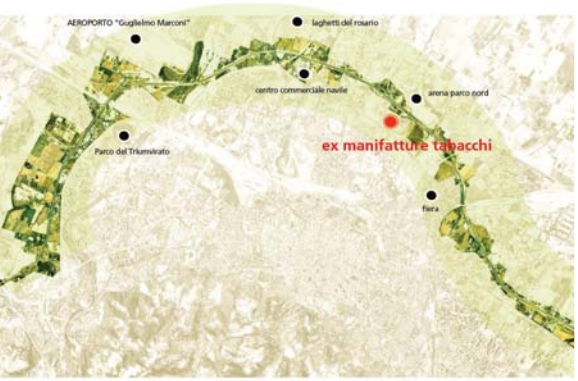
- develop a pan-European supercomputing infrastructure by acquiring and providing world-class Petascale and pre-exascale supercomputers;

- support European research and innovation activities with this HPC ecosystem, exascale and beyond, covering all scientific and industrial value chain segments.

In the short term, the JU will procure two pre-exascale systems with an expected peak performance of 250 PFlops each. An initial investment of about 1 billion euro is foreseen: about half of the sum comes from the European Commission, from actions already planned in Horizon 2020 and Connecting Europe Facility (CEF) programmes, while the remaining is to be covered by the Participating States that will host the supercomputers (hosting entites). An additional EUR ~422 millions will be contributed by private or industrial players in the form of in-kind contributions to the JU activities.
The Italian Government through an agreement signed by MIUR, CINECA, INFN and SISSA presented the Expression of Interest and proposed Cineca as hosting entity of one of the precursor of exascale supercomputers procured by the EuroHPC JU. The proposal of Italy, in consortium with Slovenia and still in evolution with Luxembourg and possibly other JU Participating States, is committed to match 120 Million Euro funded by the JU. The proposal aims to provide Europe with a system that targets the top three positions of the TOP500.
If this competition will be successful, Cineca will host the new HPC supercomputer in the Bologna Tecnopolo campus, one additional component of a wider national and regional project.
Bologna Tecnopolo campus is a set of unused buildings and grounds of a former tobacco factory (Manifattura tabacchi), built by Nervi-Bartoli from 1949. It represented a symbol of the rebirth of Bologna after World War II.
The Italian Government and Emilia Romagna Region decided to redevelop the site for hosting research laboratories on different contexts, as well as the ECMWF (European Center for Medium Range Weather Forecast) data center, the INFN Tier-1 system of the LHC experiment at CERN, and the world-level HPC center of Cineca. This will lead to the creation of one of Europe's most powerful supercomputing facilities, and a European hub for the big data processing and computing.



Bologna Science Park is the main national hub for enabling science and promoting the innovation, one of the most advanced in Europe.



Perspectives for the Italian companies competitiveness

Roberta Turra and Eric Pascolo
Cineca

Industry 4.0 represents a real revolution for the industrial world, commonly referred to as the Fourth Industrial Revolution. After the computer and automation phase of the factory, this is the era of digitalization, where the creation of a fully digital replica of the factory itself, the so called "Digital Twin", becomes possible and it can be used to predict events and optimise the production.

Industry 4.0 refers to a set of enabling technologies that allow creating applications and new services on top of classic production machines. The digital transformation brings a real advantage in competitiveness to its adopters but requires an initial investment in tools and new skills that not all companies are ready to make, especially among SMEs. To support them to undertake the process of digitization, many ongoing initiatives are ongoing at both national ad European level.

In Italy the Ministry of the Economic Development issued the National Industry 4.0 Plan (Impresa 4.0) and is now implementing the eight high specialization centers for Industry 4.0 (Competence Centers) that have been selected last June. Cineca participates to one of them, BI-REX (Big Data Innovation & Research EXcellence), which is coordinated by the University of Bologna. This Competence center, based in Bologna with 60 public and private players, is at the service of companies throughout Italy, to provide assistance and guidance in the adoption of Industry 4.0 technologies. In addition to providing a physical industrial laboratory to carry out tests and trials, BI-REX is opening 30 calls for innovation projects where companies interested in the same topic will be able to join efforts.

The calls are grouped in 8 main thematic areas: Additive and advanced manufacturing, ICT for production lines (including Edge computing, Augmented Reality, Predictive Maintenance, Precision Medicine), System integration (IoT-Cloud), Robotics, Security and blockchain, Advanced management systems of production processes (including Digital Twin), Big Data, Sustainability and social responsibility (including renewable energies).

bi-rex
Big Data Innovation & Research Excellence

At the international level, the European Commission launched the Digitise European Industry initiative. One of its pillars is digital innovation for all through Digital Innovation Hubs (DIHs), which are one-stop-shops where companies -especially SMEs, startups and mid-caps- can get help to improve their business, production processes, products and services by means of digital technology. In this context, Cineca has been acknowledged as a DIH thanks to its activity of promotion of the use of advanced technical simulations and machine learning among SMEs inside the Fortissimo EU project and I4MS (ICT Innovation for Manufacturing SMEs) initiative.

Cineca has also been recognized in 2018 as a gold label i-Space by the BDVA (Big Data Value Association). A Data Innovation Space is a cross-sectorial and cross-organizational hub that brings together data, technologies and application developments, to offer an experimentation environment to companies, with all the necessary assets to get their data-driven and AI-based services, solutions and products quickly tested, piloted and exploited.

The i-Spaces meet specific criteria in terms of quality of services and infrastructure, impact at the local and regional levels, creation and sustainability of a valuable ecosystem, and a well-defined growth and business strategy.

Projects funded under all these initiatives expose Cineca to the challenge of improving the efficiency of big data and data analytics workloads and integrating them with the simulation workloads in order to experiment hybrid approaches that integrate computational modeling with data driven modeling. The goal is to be able to provide SMEs with computational power while maintaining flexibility, in order to support innovation and to play a role in this Industry 4.0 revolution.

SCIENTIFIC OVERVIEW

Cineca is involved in many scientific fields thanks to EU projects and collaborations. From climate science to computational engineering, bioinformatics, energy and digital humanities HPC, is used to support them all.

Numerical weather prediction, from research to real-time operational applications

Davide Cesari, Thomas Gastaldo, Tiziana Paccagnella and Virginia Poli
Arpae-SIMC, Agenzia Regionale Prevenzione Ambiente Energia Emilia Romagna, Servizio Idro Meteo Clima

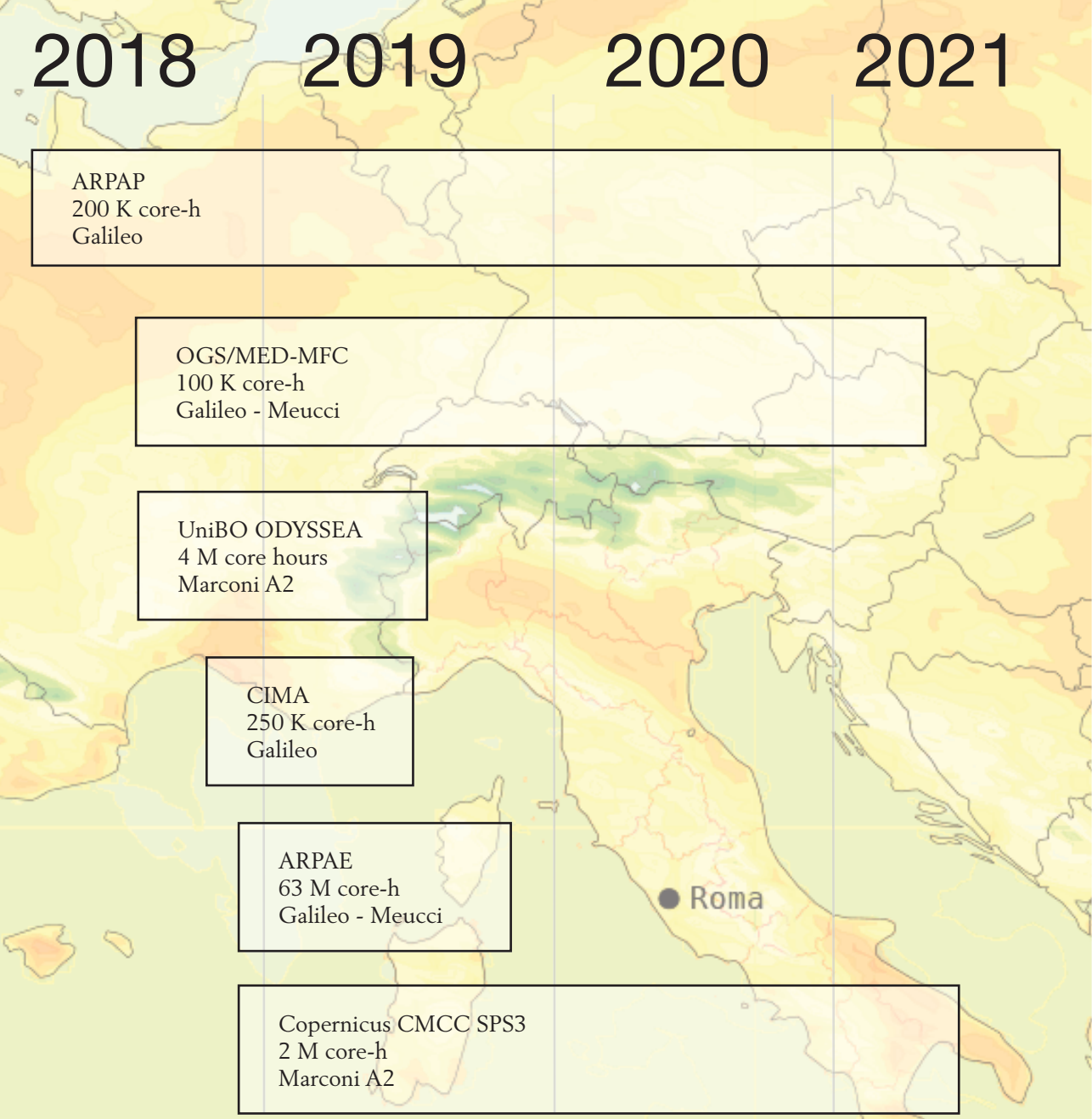
Numerical weather prediction (NWP) continuously strives to improve the quality of the meteorological models and the accuracy of the resulting meteorological forecasts. This improvement goes also through an increase of the demand for computational resources required by NWP models.

On one hand, this is due to the increase of the spatial resolution and of the complexity of forecast models themselves. In the last ten years, for example, the high resolution model run by Arpae-SIMC passed from 5 km horizontal resolution and 45 vertical levels to 2.2 km and 65 levels with an increase in the computational cost of about 20 times.

On the other hand, a great amount of computational resources is necessary to find the most accurate initial condition (analysis) from which initialize the forecast. In the NWP system in use at Arpae-SIMC this is achieved by using an ensemble Kalman filter scheme which combines meteorological observations with an ensemble of NWP model simulations. This means that, in order to produce the analysis, one model run is not sufficient anymore, but a set of runs is needed, multiplying the computational cost by the number of members of the ensemble itself. Moreover, the number of observations that can be assimilated is constantly increasing, especially thanks to satellite and radar data, and this leads to a further increase in the computational cost.

The operational assimilation system actually in use by Arpae-SIMC running on Cineca HPC system employs a 20 member ensemble and assimilates only in-situ observations. To further improve the quality of the analyses, the ensemble size should be increased to at least 40 members, in order to better represent the evolution of the atmospheric state. Furthermore, the assimilation of radar volumes over the Italian domain would be further beneficial in improving the accuracy of analyses.

Keeping in mind that the main final purpose of NWP is the emission of forecasts in real-time, with short time schedules, required in order to make the forecast usable by agencies responsible for taking measures in case of adverse weather conditions, it is clear that the use of HPC resources is essential for this purpose. Moreover, the improvement of the future accuracy of our weather forecast will be strictly linked to the improvement of the performance of the HPC system.



Starting with the Operational Activity born under the Arpa Emilia-Romagna umbrella, a lot of interesting contacts have been created and finally consolidated, aimed at the development and production of operating chains in the Meteo-Climate area.
These activities are characterized by having different computational and operational requests but represent, in total, a huge challenge for Cineca and for all the partners involved.
Some of the most relevant challenges:

- Very high SLA level (highly qualified personnel but also very resilient hardware needed)

- Daily, but also weekly and monthly execution (complicated interaction with the hardware, ad-hoc tools for production)

- Huge number of total core-hours requested (challenge for Production, it is necessary to enclose these activities in the context of PRACE, ISCRA services, ...).

In the end, meteo-climate services are targeted to be a sort of prototypes of the services that will be put on site with the upcoming National Weather Service. The role of Cineca in the field of weather-climate HPC services is therefore destined to be increasingly strategic over the next few years.

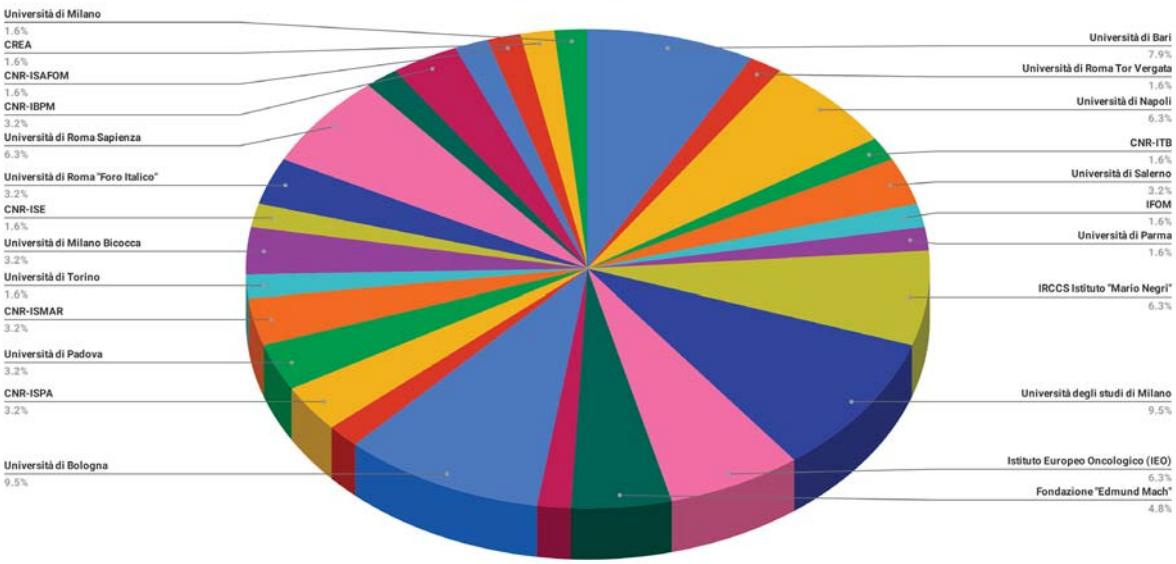
The Cineca computing service for the bioinformatics community

Tiziana Castrignanò, Silvia Gioiosa Cineca
Federico Zambelli ELIXIR-IIB and Dipartimento di Bioscienze, Università degli Studi di Milano
Giovanni Chillemi Università degli Studi della Tuscia

In the last two decades there was a vast data explosion in bioinformatics data. For this reason, the need for high-performance analysis is more pressing than ever. In particular in the area of biomedical research the volume of sequence data produced has begun to exceed the power capabilities of computer hardware employed in conventional wet laboratories as sequencing technology has improved becoming more accessible both in terms of time and money. Most of bioinformatics researchers daily process petabytes of DNA or RNA sequence data by means of advanced tools which, in turn, produce in output as much data. The HPC Department of Cineca, is the largest computing center in Italy and one of the largest in Europe. HPC Department is member of the Bioinformatics European community and has actively collaborated with the Italian scientific community in order to provide optimized software solutions for Academia and research.

The Cineca User Support Specialist team provided a rich and user friendly software environment to meet the different needs of the bioinformatics community. This provides ready access to reference data (e.g. Human, Mouse, etc.) and software tools which are regularly updated. Missing data or tools are installed on users request. Furthermore, Cineca web pipelines, implementing popular workflows for RNA-Seq (RAP[1] for transcriptome analysis, https://bioinformatics.cineca.it/rap), Exome (COVACS[2] for whole-genome, wholeexome and targeted-exome analysis, https://bioinformatics.cineca.it/covacs) and other Next Generation Sequencing data analysis are also accessibile.

References
[1] BMC Genomics. 2015 16(Suppl 6):S3 (1 June 2015) RAP: RNA-Seq Analysis Pipeline a new cloud-based NGS web application. Mattia D'Antonio, Paolo D'Onorio De Meo, Matteo Pallocca, Ernesto Picardi, Anna Maria D'Erchia, Raffaele A Calogero, Tiziana Castrignanò and Graziano Pesole.
[2] BMC Genomics 2018 19:120. 5 February 2018. CoVaCS: a consensus variant calling system. Chiara M, Gioiosa S, Chillemi G, D'Antonio M, Flati T, Picardi E, Zambelli F, Horner DS, Pesole G, Castrignanò T.



Distribution of Elixir's projects.

ELIXIR

ELIXIR (www.elixir-europe.org) is the European Research Infrastructure for biological data whose primary objective is to support research in the field of "life sciences" and their translational activities to medicine, environment, biotechnological industries and society.

ELIXIR is structured as a central hub, located in the Wellcome Genome Campus (Hinxton, UK) and 20 national nodes including over 160 Research Organizations.

The Italian node ELIXIR-IIB (http://elixiritaly.org/en/) is a full member of ELIXIR since 2016, after the signature by MIUR of the ELIXIR Consortium Agreement. It is led by Italian National Research Council (CNR) and it is configured as a Joint Research Unit (JRU) which coordinates the delivery of existing bioinformatics services at a national level, also pursuing their integration in the ELIXIR infrastructure. Cineca is one of the technological partners of ELIXIR-IIB.

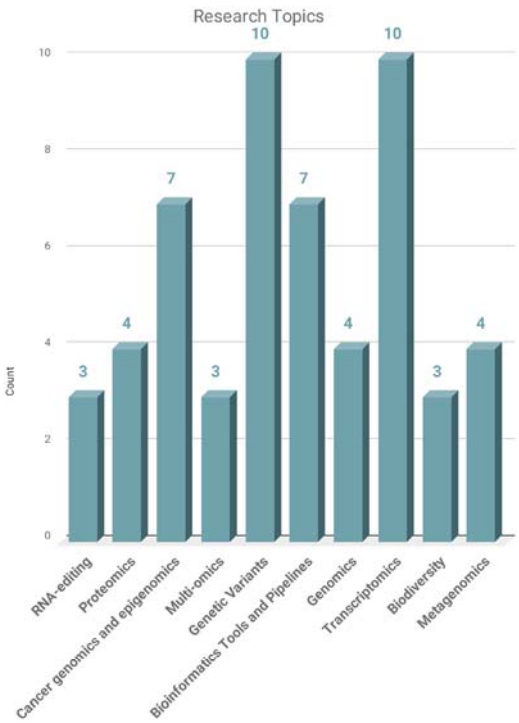
In April 2016 the Italian node of ELIXIR and Cineca started the ELIXIR-IIB HPC@CINECA Call, in order to offer computational resources to researchers from ELIXIR-IIB, other ELIXIR Nodes and any European research institution.

Resources are provided through web interfaces to the Cineca bioinformatics pipeline or command line over Unix environment on the Cineca High Performance Computing platforms. Project proposals are evaluated by an ELIXIR-IIB Review Committee that checks their scientific and technical soundness through a fast procedure following a "first come, first served" policy.

Up to now, three millions of core hours were distributed to nearly 50 bioinformatic projects.

The first two years on the "Pico" cluster and lately on the "New Galileo" cluster (composed by 360x36-core compute nodes, each one containing 2x18-cores Intel Xeon E5-2697 v4 Broadwell @2.30 GHz. All the compute nodes have 128 GB of memory. 15 of these compute nodes are equipped with two nVidia K80 GPU).

The Cineca User Support Specialist team provided a rich and user friendly software environment to meet the different needs of the bioinformatics community. This provides ready access to reference data (e.g. Human, Mouse, etc.) and software tools which are regularly updated. Missing data or tools are installed on users request. Furthermore, Cineca web pipelines, implementing popular workflows for RNA-Seq (RAP[1] for transcriptome analysis, https://bioinformatics.cineca.it/rap), Exome (COVACS[2] for whole-genome, wholeexome and targeted-exome analysis, https://bioinformatics.cineca.it/covacs) and other Next Generation Sequencing data analysis are also accessibile.

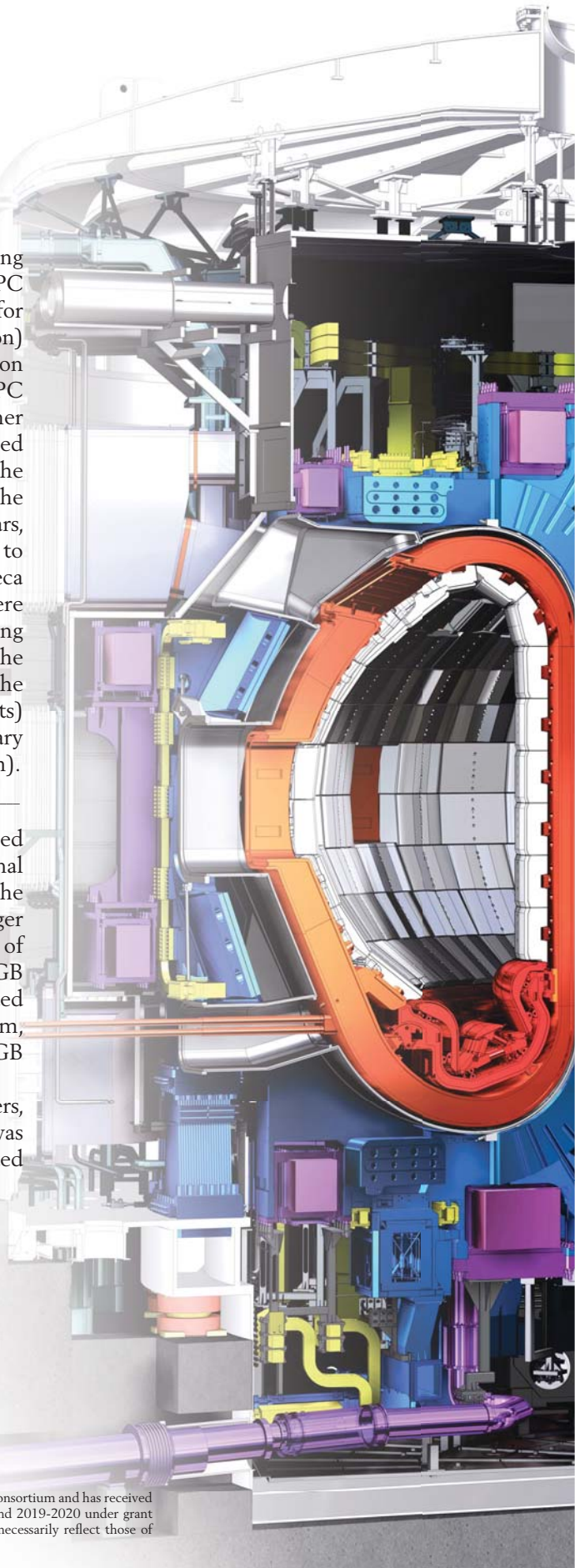


Energy

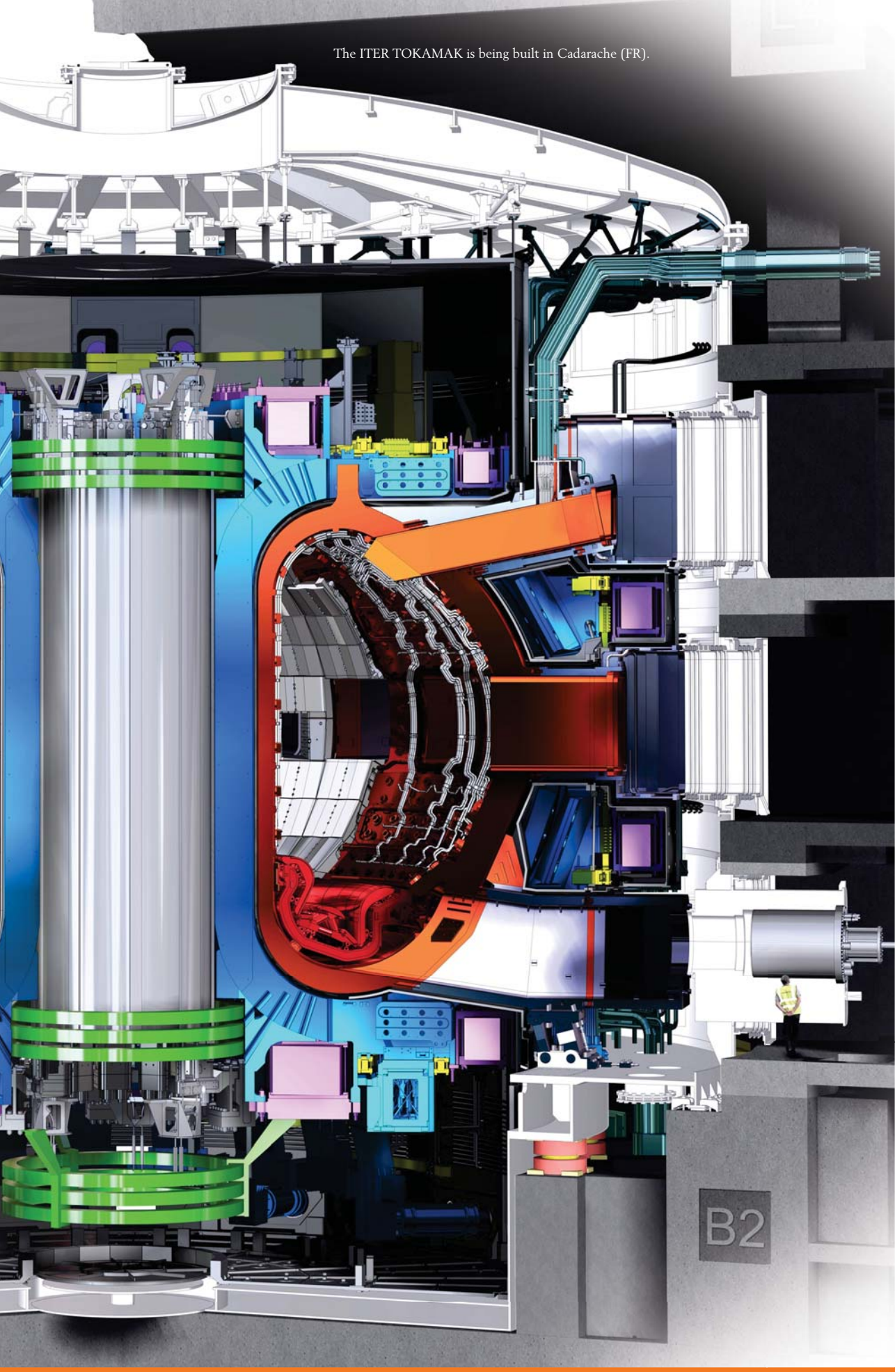
Elda Rossi
Cineca

In the 2016, another important HPC operating service was added under Cineca HPC responsibility. The European Consortium for Development of Fusion Energy (EUROfusion) decided by mean of an international selection to entrust their simulations to Cineca's HPC infrastructures. During 2018 after another international selection, EUROfusion confirmed the confidence in Cineca renewing the collaboration for two more years, with the possibility of an extension of three more years, till 2023 for HPC access service. In order to satisfy the requirements of Eurofusion, Cineca designed and selected infrastructures where the plasma physics simulations run, optimizing their performances and the stability of the starting environment, after the migration of the production from Japan (for the computing parts) and from Germany (for the complementary tools, and services hosted gateway server farm).

In year 2018, the HPC infrastructure reserved to EUROfusion consisted in one conventional partition, and one accelerated partition. The conventional partition was part of the larger Marconi system, consisting in 1528 nodes of SKL technology, each node composed of 256 GB of shared memory and 48 cores. The accelerated partition too is hosted on the Marconi system, about 400 KNL nodes, 68 cores sharing a 96 GB memory, the so-called many-core technology.
In addition to these HPC production clusters, an interactive system called "Gateway" was available for the EUROfusion users interested in code developing.



This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.



The ITER TOKAMAK is being built in Cadarache (FR).

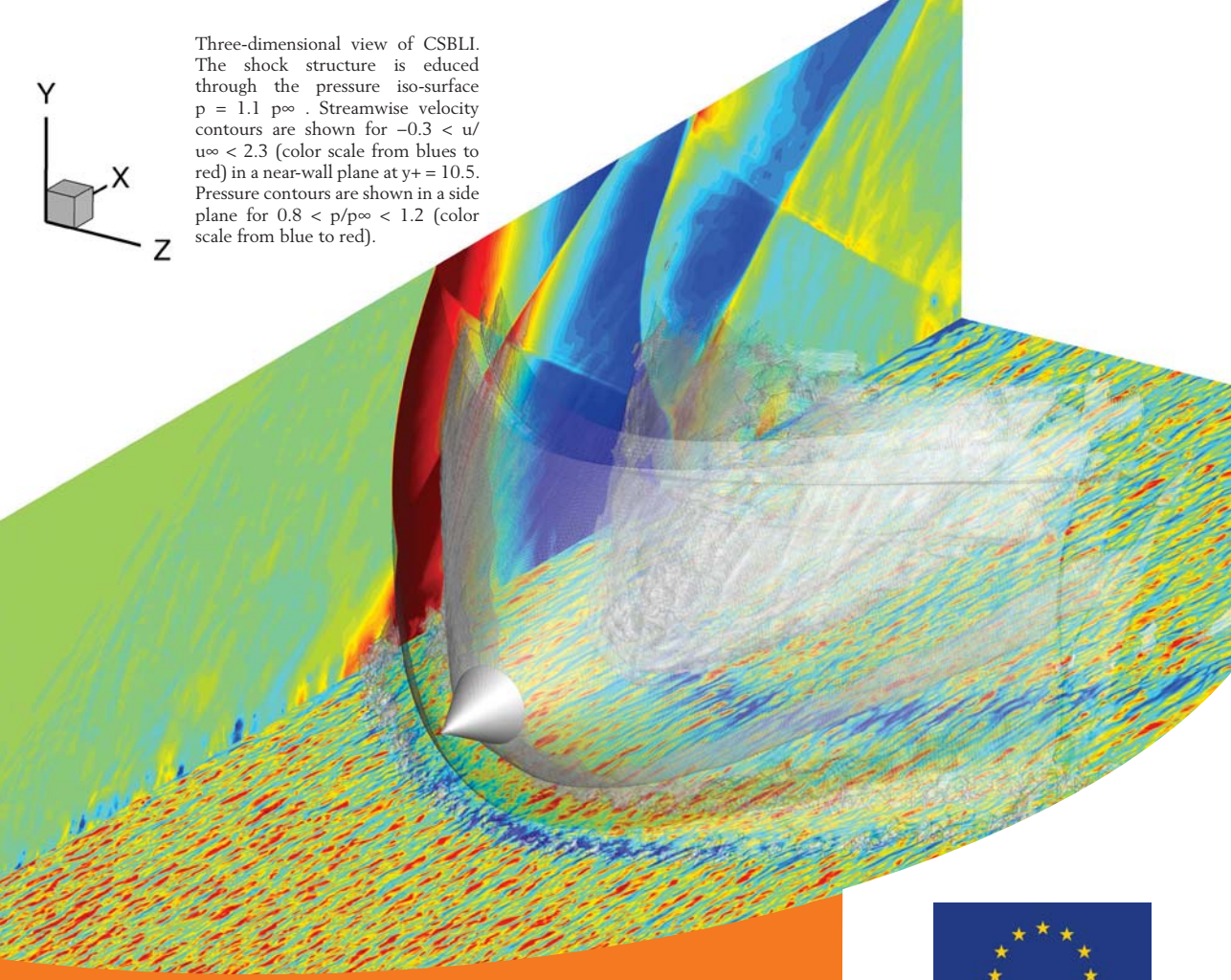
Aeronautics and aerospace engineering
Numerical simulations of three-dimensional shock/boundary layer interactions

Sergio Pirozzoli, Antonio Memmolo
Dipartimento di Ingegneria Meccanica e Aerospaziale, Sapienza Università di Roma
Feng-Yuan Zuo
College of Energy and Power Engineering, Nanjing University of Aeronautics and Astronautics, China

Shock wave/turbulent boundary layer interactions (SBLI) have great relevance in aeronautics and aerospace engineering, being encountered whenever a shock wave sweeps across the boundary layer developing on a solid surface. SBLI are for instance found in wing-fuselage and tail-fuselage junctions of aircraft, helicopter rotors, supersonic air intakes, over-expanded nozzles, launch vehicles during the ascent phase. SBLI may have a significant drawback on aerodynamic performance, yielding loss of efficiency of aerodynamic surfaces, unwanted wall pressure fluctuations possibly leading to structural vibrations, and localized heat transfer peaks, especially in presence of flow separation. To date, most studies of SBLI have been carried out in idealized settings involving geometrically two-dimensional configurations, and/or using simplified modeling approaches. However, SBLI occurring in flow conditions of practical relevance are almost invariably three-dimensional in nature, a prominent case being that in which the shock wave has a conical shape (CSBLI), as in supersonic body/body interference problems. Spanwise non-uniformity of the imposed pressure gradient makes this flow hard to predict for engineering turbulence models in current use, and use of advanced techniques as Direct Numerical Simulation (DNS) is expected to yield a boost to the development of improved prediction models.

DNS consists in the direct solution of the Navier-Stokes equations in their unsteady, three-dimensional form, with a mesh capable of resolving even the smallest involved scales of motion (eddies). Besides the need for highly accurate discretization algorithms, the main challenge in DNS is of computational nature, as a huge number of grid points (typically, in the order of hundreds of millions to several billions), as well as steps in time are required. Extreme computational intensity is further exacerbated in CSBLI by the totally inhomogeneous nature of turbulence, which slows down statistical convergence of the computations. Clearly, access to large HPC systems is the only viable path to achieve the research goals in reasonable time.

The group led by Prof. Pirozzoli has long experience in the numerical simulation of compressible turbulent flows, as well as supercomputing on Cineca machines, using ISCRA and PRACE grants. The solver to be used for the analysis has been extensively optimized with the help of Cineca staff, and parallel scalability up to 16384 has been obtained. Preliminary results of the DNS study are shown in Figure 1, in which the shock generated by a cone with opening angle of 25° at Mach number 2 impacts on a turbulent boundary layer underneath. DNS allows to analyze in their full complexity the flow patterns resulting from CSBLI. The database thus obtained is currently being mined, with the main objective of deriving improved turbulence models capable of accounting for cross-stream pressure gradient at higher Reynolds number.



Three-dimensional view of CSBLI. The shock structure is educed through the pressure iso-surface $p = 1.1\ p_\infty$. Streamwise velocity contours are shown for $-0.3 < u/u_\infty < 2.3$ (color scale from blues to red) in a near-wall plane at $y+ = 10.5$. Pressure contours are shown in a side plane for $0.8 < p/p_\infty < 1.2$ (color scale from blue to red).

Cineca's innovation EU projects

The ICARUS project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 780792.

The LINCOLN project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 727982.

The PRACE-5IP project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No EINFRA-730913.

The Fortissimo 2 project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 680481.

EOSC-hub receives funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 777536.

Complexity and data
New Deep Learning architectures and computer vision for image and video understanding

Lorenzo Baraldi and Rita Cucchiara
Aimagelab, Università di Modena e Reggio Emilia

AImageLab is a research laboratory at the University of Modena and Reggio Emilia which covers topics of Computer Vision, Pattern Recognition, Machine Learning, AI and Multimedia. AImageLab accounts about 25 researchers working in European, National and Regional projects as well as many industrial research projects funded by industries and institutions (see aimagelab.unimore.it).
In the last three years, AImageLab has focused most of research activities on developing new Deep Learning architectures and data-intensive Computer Vision approaches, which require adequate computational capabilities to train neural networks with millions of learnable parameters.
To satisfy such computational needs, over the years we have built a two-layer GPU-based computing environment which interacts with the facilities at Cineca. At the lowest level, researchers at AImageLab can build and train small-scale and medium-scale research prototypes exploiting the on-site available GPU resources (more than 300TFlops available on local servers with NVIDIA GPUs) at the highest level, instead, long-running and intensive experiments are seamlessly transferred to one of the Cineca supercomputers. From a technical perspective, both layers exploit the same queue management system that Cineca has adopted (i.e. SLURM), thus guaranteeing simplicity of use and a uniform user experience which ultimately results in higher research throughput.
While most of the research activities carried out at AImageLab have high computational demand, here we focus on three of the most computationally intensive, i.e. the description of images in natural language, the analysis of videos, and the applications to cultural heritage.

DESCRIBING IMAGES IN NATURAL LANGUAGE

AImageLab has developed image and video captioning algorithms which can automatically describe the visual content in natural language, thus connecting vision and language as our brain does. Most of the developed architectures rely on the combination of Convolutional and Recurrent Networks [1, 2], which are trained on large-scale datasets with millions of samples. Research on this field is carried out both at the architectural level, defining and testing novel recurrent cells and integrating training strategies based on Reinforcement Learning, and at the feature level, investigating more effective ways of extracting the content of images and videos. For both lines of work, high computational capabilities and high parallelism are required to investigate the possible design choices in reasonable time. For this reason, we have tested and exploited the newborn D.A.V.I.D.E. platform, which offers state of the art GPUs and high parallelism.

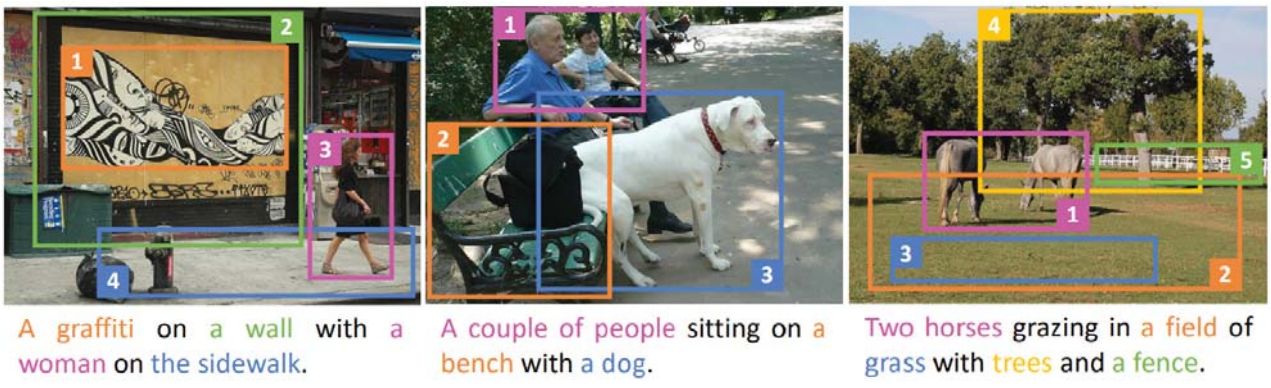


Figure 1: Captions automatically generated from sample images.

ANALYZING VIDEOS AND ACTIONS

A second research line deals with the automatic comprehension of videos, with applications such as video summarization, tagging and retrieval [3, 4]. In this context, AimageLab has developed innovative solutions for decomposing and summarizing the storytelling structure of videos, during a national PON-PNR research project "Città Educante" in which we cooperated with RAI on the analysis of broadcast videos, and in collaboration with Facebook AI Research for investigating novel descriptors for video retrieval. As naturally happens when dealing with the exploding high dimensionality of videos, high-performance computing is fundamental to investigate different solutions: in this case, we have exploited thousands of core-hours on the Galileo platform to process videos from the RAI archive.

Figure 2: NeuralStory - a platform for video browsing, summarization, and re-use.

SEEING WITH ART: CULTURAL HERITAGE APPLICATIONS

Many of the approaches developed at AImageLab have also been applied to art and to the domain of Digital Humanities. This is the case of networks which can predict the human gaze[5] and the areas of attention of a painting, or which can retrieve sculptures from textual queries. As applying state-of-art Neural Networks to painting can be difficult, due to the difference of texture with natural images, we have also developed architectures which can translate paintings to photorealistic visualizations, thus easing the automatic extraction of knowledge from artistic data. Also in this case, the D.A.V.I.D.E. platform has been exploited to train Generative Adversarial Networks directly on CPU, thus increasing the output size of the generated visualizations.

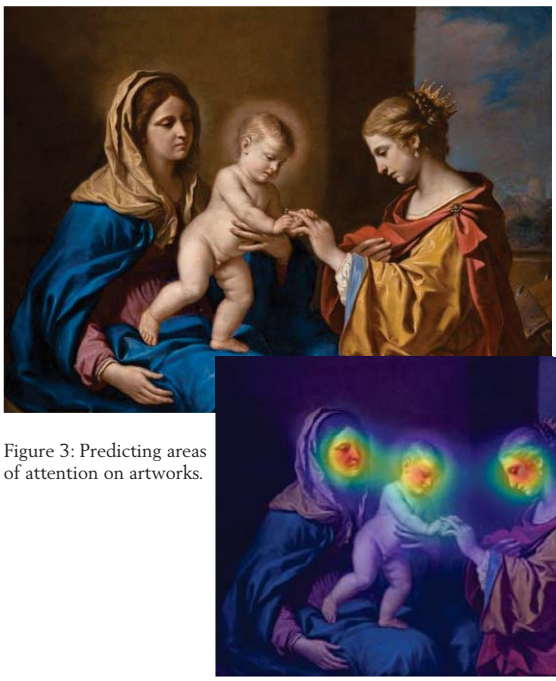


Figure 3: Predicting areas of attention on artworks.

References

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[2] Cornia, Marcella, Lorenzo Baraldi, and Rita Cucchiara. "Show, Control and Tell: A Framework for Generating Controllable and Grounded Captions." arXiv preprint arXiv:1811.10652

[3] Baraldi, Lorenzo; Douze, Matthijs; Cucchiara, Rita; Jégou, Hervé "LAMV: Learning to align and match videos with kernelized temporal layers", CVPR 2018

[4] Baraldi, Lorenzo; Grana, Costantino; Cucchiara, Rita "Recognizing and Presenting the Storytelling Video Structure with Deep Multimodal Networks" IEEE Transactions on Multimedia, 2016

[5] Cornia, Marcella; Baraldi, Lorenzo; Serra, Giuseppe; Cucchiara, Rita "Predicting Human Eye Fixations via an LSTM-based Saliency Attentive Model" IEEE Transactions on Image Processing, 2018

Figure 4: Generating photo-realistic visualization from paintings.

Digital Humanities

Mauro Felicori
Responsabile progetto AGO, Fondazione Cassa di Risparmio di Modena
Antonella Guidazzoli
Cineca

Since 2016 a fruitful collaboration is going on between Cineca and Caserta Royal Palace for promoting its Heritage by leveraging on big data, sentiment analysis and 3D applications. The first output was a 3DWeb virtual installation that allows visitors to remotely visit the Terra Motus exhibition, a physical set up opened in 2016 at the Royal Palace of Caserta (https://goo.gl/wsyRYR). The virtual exhibition, as a web application, allows interested people to live the Terrae Motus exhibition in a visualization similar to that of an interactive video game, directly within any Web browser, without the need to install any additional plug-in, on any device, such as PC, tablet and smartphone. The technology is based on Blend4Web: an effective tool that allows the export of Blender contents to web pages and provides a WebGL rendering, as well as audio support, animations and programmable user interaction.

Tourism, as an emotional experience, increasingly relies for its promotion on social media, making the sentiment analysis a powerful tool for deciphering feelings and opinions of actual and possible visitors. The sentiment analysis realized by HPC Department in 2018 has noted that Internet users appreciated the social network profiles of Caserta Royal Palace more than ever. The new website, a new marketing strategy with several events and collaborations with local authorities, more attention to social networks, as a tool for information and tourist promotion, gave to Caserta Royal Palace +60.000 likes on Facebook, +4.400 followers on Twitter, +1600 reviews on Tripadvisor. All of this materialized with an increase in visitors of around 23%. The research numbers say that over half of the total interactions recorded on social media (posts, tweets and reviews) have a positive sentiment towards the Palace, with an average value in the last 3 years equal to 74 (on a scale from 0 to 100). The Facebook sentiment is higher (80), slightly lower the values of Twitter (73) and Tripadvisor (70). The effects of this strategy had an important echo also abroad, both inside the "museum system" (from 47 in 2015 to 85 in 2017), and among visitors, with an increase in sentiment associated with their visits (from 70 to 74).

Cineca also supported the Royal Palace involvement in the World Heritage Journeys Europe platform. Launched in September 2018, the platform was created by National Geographics under a EU Commission input to channel the tourist flows coming from North America and China to the European sites included in the UNESCO World Heritage List (www.visitworldheritage.com/en/eu). The website experienced a significant growth in traffic following the programme launch, primarily as a result of extensive media coverage. During the first three months (October -December 2018) just over 36% of website traffic originates in China, while the US, France, Italy, Spain and Germany each account for about 5% of total traffic. About 90% of website users are visiting the site for the first time. For its part, the Royal Palace chose to widen the boundaries of the communication through this promotional opportunity, ideally embracing all the immense material and immaterial heritage present in the area nearby (#neidintornidellareggia) to parade both the Reggia and its territory.

Commissioned by the Museum of the New Towns, "Il piccolo Masaccio e le Terre Nuove" is a short animated Computer Graphics educational movie, developed at VisitLab Cineca and mainly intended for the younger audience of the museum (video trailer at https://youtu.be/JwdKB_xchF8). The video presents a series of very different technical solutions, such as: live shots, taken also by drone; 2D drawings executed with a digital tablet; drawings sketched with traditional techniques, such as India ink and watercolours; traditional and procedural 3D modelling; photogrammetry, also for textures; crowd, cloth and particle simulations; a digital library for the vegetation of the time; digital videos taken from Google Earth.
Created in Blender 2.78 - 2.79 and rendered with Cycles render engine, the video heavily relied on supercomputing for the rendering phase, both during its development and the final high res version. Blender Render Farm on Supercomputer Galileo (360 Compute nodes (Intel Broadwell), each with 2*18-core Intel Xeon E5-2697 v4 @ 2.30GHz - 128 GB RAM).

150.000 core hours
for rendering both low and high quality frames

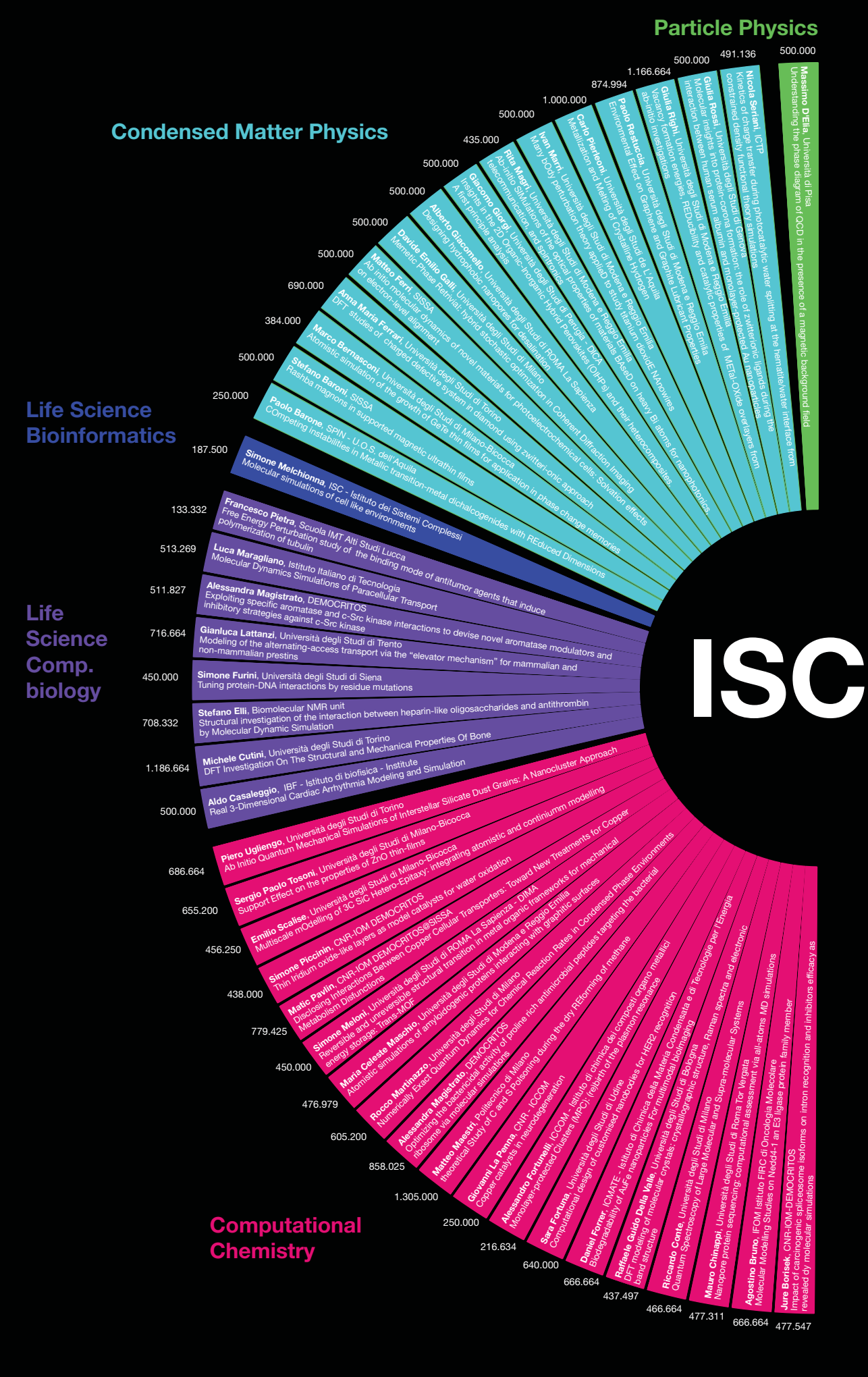
15 GB
high resolution frames

15,3 GB
Blender files and textures

Terraemotus VR application - collaborative environment.

USERS' PROJECTS

Three different programmes are available to offer computational resources to researches, based on a peer-review access: Prace, at the European level; Iscra, at the national level; Lisa, funded by Regione Lombardia and restricted to researchers working in the area.
In the following, some exemplary projects granted in 2018 are presented.


Particle Physics
Condensed Matter Physics
Life Science Bioinformatics
Life Science Comp. biology
Computational Chemistry
ISC
500.000
Massimo D'Elia, Università di Pisa
Understanding the phase diagram of QCD in the presence of a magnetic background field
491.136
Nicola Seriani, ICTP
Kinetics of charge transfer during photocatalytic water splitting at the hematite/water interface from constrained density functional theory simulations
500.000
Giulia Rossi, Università degli Studi di Genova
Molecular insights into protein-corona formation: the role of zwitterionic ligands during the interaction between human serum albumin and monolayer-protected Au nanoparticles
1.166.664
Giulia Righi, Università degli Studi di Modena e Reggio Emilia
Vacancy formation energies, REDucibility and catalytic properties of METal-OXide overlayers from ab-initio investigations
874.994
Paolo Restuccia, Università degli Studi di L'Aquila
Environmental Effect on Graphene and Graphite Lubricant Properties
1.000.000
Carlo Pierleoni, Università degli Studi di Modena e Reggio Emilia
Metallization and Melting of Crystalline Hydrogen
500.000
Ivan Marri, Università degli Studi di Modena e Reggio Emilia
Many body perturbation theory applieD to study titanium dioxidE NAnowires
435.000
Rita Magri, Università degli Studi di Modena e Reggio Emilia
Ab-Initio SIMulations of the optical properties of materials: BAseD on heavy Bi atoms for nanophotonics
500.000
Giacomo Giorgi, Università degli Studi di Perugia DICA
Insights in the 2D Organic-Inorganic Hybrid Perovskites (OIHPs) and their heterocomposites
500.000
Alberto Giacomello, Università degli Studi di ROMA La Sapienza
Designing hydrophobic nanopores for desalination
500.000
Davide Emilio Galli, Università degli Studi di Milano
A first principle analysis of Coherent Diffraction Imaging
500.000
Matteo Farè, SISSA
Ab initio molecular dynamics of novel materials for photoelectrochemical cells: Solvation effects on electron-level alignment
690.000
Anna Maria Ferrari, Università degli Studi di Torino
Mimetic Phase Retrival: hybrid stochastic optimization in Coherent Diffraction Imaging
384.000
Marco Bernasconi, Università degli Studi di Milano-Bicocca
DFT studies of charged defective system in diamond using zwitteri-onic approach
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Stefano Baroni, SISSA
Atomistic simulation of the growth of GeTe thin films for application in phase change memories
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Paolo Barone, SPIN - U.O.S. dell'Aquila
Rashba magnons in supported magnetic ultrathin films
187.500
Simone Melchionna, ISC - Istituto dei Sistemi Complessi
COmpeting instabilities in Metallic transition-metal dichalcogenides with REduced Dimensions
133.332
Francesco Pietra, Scuola IMT Alti Studi Lucca
Molecular simulations of cell like environments
513.269
Luca Maragliano, Istituto Italiano di Tecnologia
Free Energy Perturbation study of the binding mode of antitumor agents that induce polymerization of tubulin
511.827
Alessandra Magistrato, DEMOCRITOS
Molecular Dynamics Simulations of Paracellular Transport
716.664
Gianluca Lattanzi, Università degli Studi di Trento
Exploiting specific aromatase and c-Src kinase interactions to devise novel aromatase modulators and inhibitory strategies against c-Src kinase
450.000
Simone Furini, Università degli Studi di Siena
Modeling of the alternating-access transport via the "elevator mechanism" for mammalian and non-mammalian prestins
708.332
Stefano Elli, Biomolecular NMR unit
Tuning protein-DNA interactions by residue mutations
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Michele Cutini, Università degli Studi di Torino
Structural investigation of the interaction between heparin-like oligosaccharides and antithrombin by Molecular Dynamic Simulation
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Aldo Casaleggio, IBF - Istituto di biofisica - Institute
DFT Investigation On The Structural and Mechanical Properties Of Bone
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Piero Ugliengo, Università degli Studi di Torino
Real 3-Dimensional Cardiac Arrhythmia Modeling and Simulation
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Sergio Paolo Tosoni, Università degli Studi di Milano-Bicocca
Ab Initio Quantum Mechanical Simulations of Interstellar Silicate Dust Grains: A Nanocluster Approach
456.250
Emilio Scalise, Università degli Studi di Milano-Bicocca
Support Effect on the properties of ZnO thin-films
438.000
Simone Piccinin, CNR-IOM DEMOCRITOS
Multiscale mOdelling of 3C SiC Hetero-Epitaxy: Integrating atomistic and continuum modelling
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Thin Iridium oxide-like layers as model catalysts for water oxidation
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Simone Meloni, Università degli Studi di ROMA La Sapienza - DIMA
Disclosing Interactions Between Copper Cellular Transporters: Toward New Treatments for Copper Metabolism Disfunctions
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Maria Celeste Maschio, Università degli Studi di Modena e Reggio Emilia
Reversible and unreversible structural transition in metal organic frameworks for mechanical energy storage: Trans-MOF
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Rocco Martinazzo, Università degli Studi di Milano
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Sara Fortuna, Università degli Studi di Udine
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Daniel Forrer, ICMATE - Istituto di Chimica della Materia Condensata e di Tecnologie per l'Energia
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Raffaele Guido Della Valle, Università degli Studi di Bologna
Biodegradability of AuFe nanoparticles For multimodal bioimaging
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Riccardo Conte, Università degli Studi di Milano
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Mauro Chinappi, Università degli Studi di Roma Tor Vergata
Quantum Spectroscopy of Large Molecular and Supra-molecular Systems
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Agostino Bruno, IFOM Istituto FIRC di Oncologia Molecolare
Nanopore protein sequencing: computational assessment via all-atoms MD simulations
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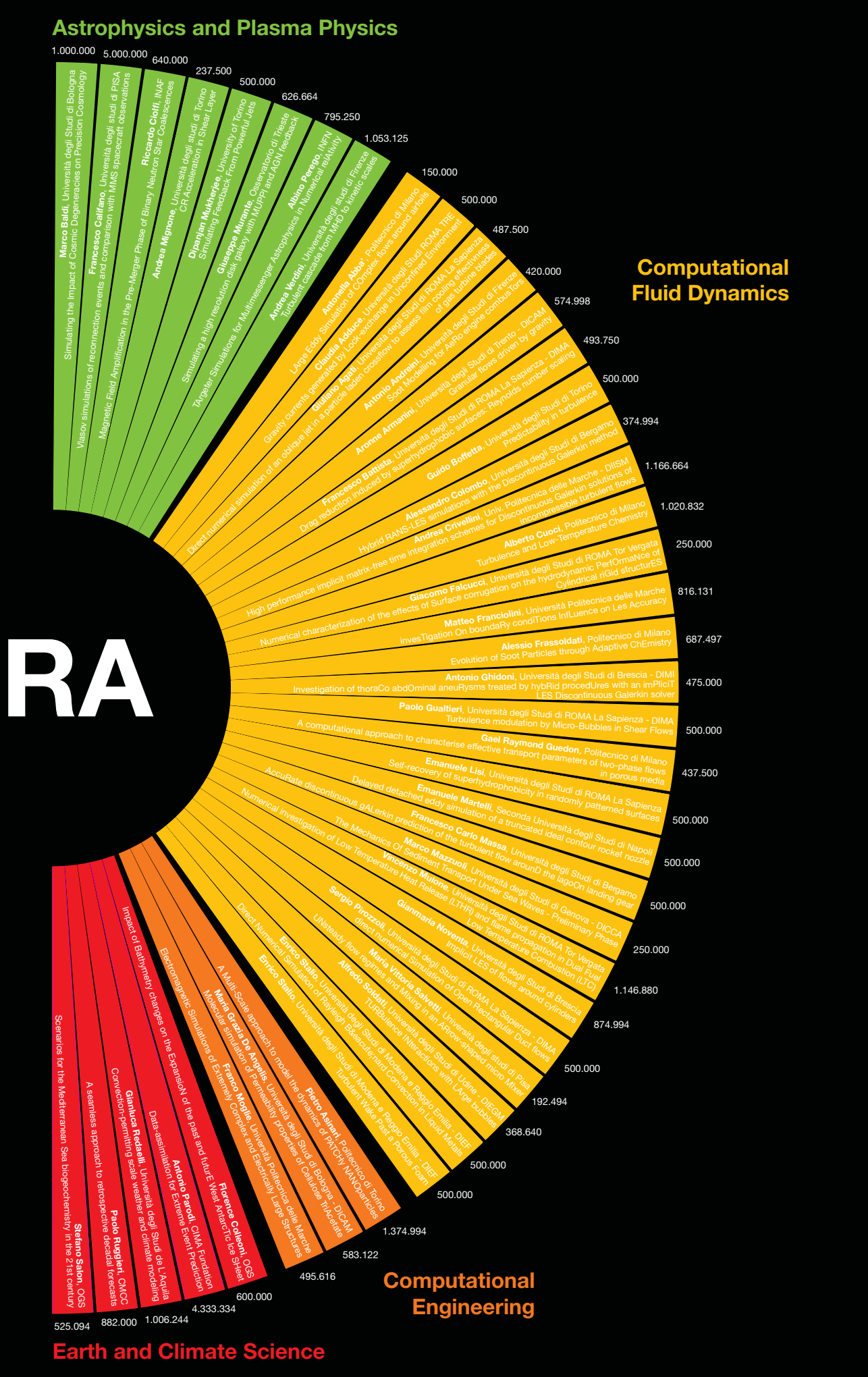
Impact of carcinogenic spliceosome isoforms on intron recognition and inhibitors efficacy as revealed dy molecular simulations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Giuseppe Murante, Osservatorio di Trieste
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Albino Perego, INFN
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Antonella Abbà, Politecnico di Milano
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Claudia Adduce, Università degli Studi ROMA TRE
Gravity currents generated by Lock-exchange in Unconfined Environment
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Giuliano Agati, Università degli Studi di ROMA La Sapienza
Direct numerical simulation of an oblique jet in a particle laden crossflow to assess film cooling effectiveness
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Antonio Andreini, Università degli Studi di Firenze
Soot Modeling for AeRo engine combustors
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Granular flows driven by gravity
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Francesco Battista, Università degli Studi di ROMA La Sapienza - DIMA
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Predictability in turbulence
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invesTigation On boundaRy condiTions IntLuence on Les Accuracy
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Turbulence modulation by Micro-Bubbles in Shear Flows
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Gael Raymond Guedon, Politecnico di Milano
A computational approach to characterise effective transport parameters of two-phase flows in porous media
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Emanuele Martelli, Seconda Università degli Studi di Napoli
Delayed detached eddy simulation of a truncated ideal contour rocket nozzle
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Francesco Carlo Massa, Università degli Studi di Bergamo
Accurate discontinuous gALerkin prediction of the turbulent flow arounD the lagoOn landing gear
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Direct numerical Simulation of Open Rectangular Duct flows
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Gianmaria Noventa, Università degli Studi di Brescia
Implicit LES of flows around cylinders
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Marta Vittoria Salvetti, Università degli studi di Pisa
UNsteady flow regimes and MIxing in an ARrow-shaped micro MIxer
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Alfredo Soldati, Università degli Studi di Udine - DIEGM
TUrbulence INteractions with LArge bubbles
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Enrico Stalio, Università degli Studi di Modena e Reggio Emilia - DIEF
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Turbulent Wake Past a Porous Foam
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Computational Engineering
Pietro Asinari, Politecnico di Torino
A Multi-Scale approach to model the dynamics of PATCHy NANOparticles
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Maria Grazia De Angelis, Università degli Studi di Bologna - DICAM
Molecular simulation of Permeability properties of Cellulose TriAcetate
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Franco Miglio, Università Politecnica delle Marche
Electromagnetic Simulations of Extremely Complex and Electrically Large Structures
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Florence Colleoni, OGS
Impact of Bathymetry changes on the ExpansioN of the past and futurE West Antarctic Ice Sheet
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Antonio Parodi, CIMA Fundation
Data-assimilation for Extreme Event Prediction
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Gianluca Redaelli, Università degli Studi de L'Aquila
Convection-permitting scale weather and climate modeling
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Paolo Ruggieri, CMCC
A seamless approach to retrospective decadal forecasts
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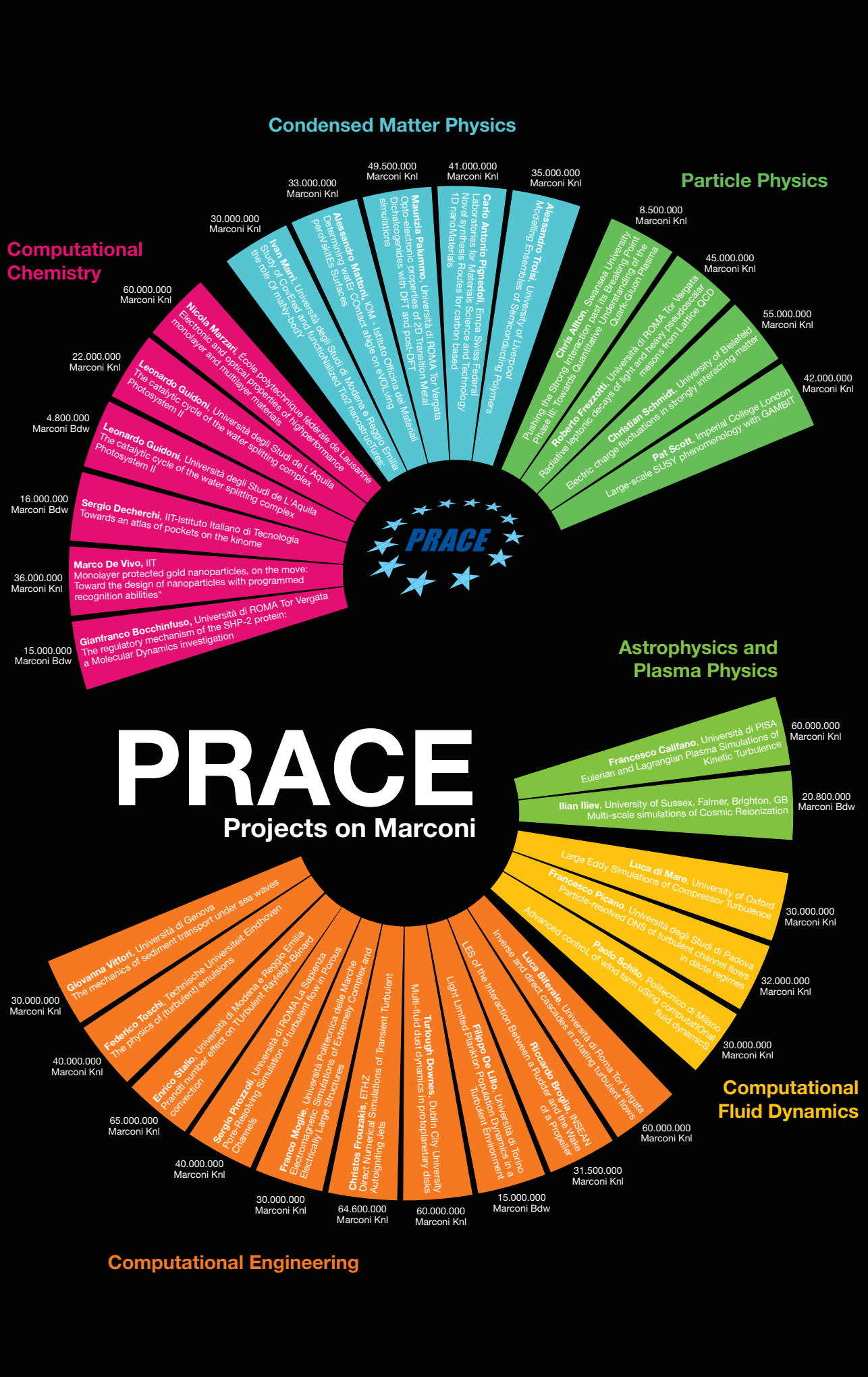
Stefano Salon, OGS
Scenarios for the Mediterranean Sea biogeochemistry in the 21st century
Earth and Climate Science
RA


PRACE
Projects on Marconi
Condensed Matter Physics
Particle Physics
Computational Chemistry
Astrophysics and Plasma Physics
Computational Fluid Dynamics
Computational Engineering
Alessandro Troisi, University of Liverpool Modelling Ensembles of Semiconducting Polymers 35.000.000 Marconi Knl
Carlo Antonio Pignedoli, Empa Swiss Federal Laboratories for Materials Science and Technology Novel synthesis Routes for carbon based 1D nanoMaterials 41.000.000 Marconi Knl
Maurizia Palummo, Università di ROMA Tor Vergata Opto-electronic properties of 2D Transition Metal Dichalcogenides with DFT and post-DFT simulations 49.500.000 Marconi Knl
Alessandro Mattoni, IOM - Istituto Officina dei Materiali Determining wat.Er COntact angle on eVOLving perovSkiTES Surfaces 33.000.000 Marconi Knl
Ivan Marri, Università degli Studi di Modena e Reggio Emilia Study of CoVErEd and funcNoNalized TroZ nanostructures: the role Of manY-body 30.000.000 Marconi Knl
Chris Allton, Swansea University Pushing the Strong Interaction past its Breaking Point phase III: Towards Quantitative Understanding of the Quark-Gluon Plasma 8.500.000 Marconi Knl
Roberto Frezzotti, Università di ROMA Tor Vergata Radiative leptonic decays of light and heavy pseudoscalar mesons from Lattice QCD 45.000.000 Marconi Knl
Christian Schmidt, University of Bielefeld Electric charge fluctuations in strongly interacting matter 55.000.000 Marconi Knl
Pat Scott, Imperial College London Large-scale SUSY phenomenology with GAMBIT 42.000.000 Marconi Knl
Nicola Marzari, École polytechnique fédérale de Lausanne Electronic and optical properties of high-performance monolayer and multilayer materials 60.000.000 Marconi Knl
Leonardo Guidoni, Università degli Studi de L'Aquila The Catalytic cycle of the water splitting complex Photosystem II 22.000.000 Marconi Knl
Leonardo Guidoni, Università degli Studi de L'Aquila The catalytic cycle of the water splitting complex Photosystem II 4.800.000 Marconi Bdw
Sergio Decherchi, IIT-Istituto Italiano di Tecnologia Towards an atlas of pockets on the kinome 16.000.000 Marconi Bdw
Marco De Vivo, IIT Monolayer protected gold nanoparticles, on the move: Toward the design of nanoparticles with programmed recognition abilities* 36.000.000 Marconi Knl
Gianfranco Bocchinfuso, Università di ROMA Tor Vergata The regulatory mechanism of the SHP-2 protein: a Molecular Dynamics investigation 15.000.000 Marconi Bdw
Francesco Califano, Università di PISA Eulerian and Lagrangian Plasma Simulations of Kinetic Turbulence 60.000.000 Marconi Knl
Ilian Iliev, University of Sussex, Falmer, Brighton, GB Multi-scale simulations of Cosmic Reionization 20.800.000 Marconi Bdw
Luca di Mare, University of Oxford Large Eddy Simulations of Compressor Turbulence
Francesco Picano, Università degli Studi di Padova Particle-resolved DNS of turbulent channel flows in dilute regimes 30.000.000 Marconi Knl
Paolo Schito, Politecnico di Milano Advanced control of wind farm using computational fluid dynamics 32.000.000 Marconi Knl
Luca Biferale, Università di Roma Tor Vergata Inverse and direct cascades in rotating turbulent flows 30.000.000 Marconi Knl
Riccardo Broglia, INSEAN Flow around a Rudder and the Wake of a Propeller 60.000.000 Marconi Knl
Filippo De Lillo, Università di Torino LES of the Interaction Between a Turbulent Environment 31.500.000 Marconi Knl
Turlough Downes, Dublin City University Multi-fluid dust dynamics in protoplanetary disks 15.000.000 Marconi Bdw
Christos Frouzakis, ETHZ Direct Numerical Simulations of Transient Turbulent Autoignition Jets 60.000.000 Marconi Knl
Franco Moglie, Università Politecnica delle Marche Electromagnetic Simulations of Extremely Complex and Electrically Large Structures 64.600.000 Marconi Knl
Sergio Pirozzoli, Università di ROMA La Sapienza Pore-Resolving Simulation of turbulent flow in Porous Channels 30.000.000 Marconi Knl
Enrico Stalio, Università di Modena e Reggio Emilia Prandtl number effect on TUrbulent Rayleigh-Bénard convection 40.000.000 Marconi Knl
Federico Toschi, Technische Universiteit Eindhoven The physics of (turbulent) emulsions 65.000.000 Marconi Knl
Giovanna Vittori, Università di Genova The mechanics of sediment transport under sea waves 30.000.000 Marconi Knl

High Performance Computing for fracking application

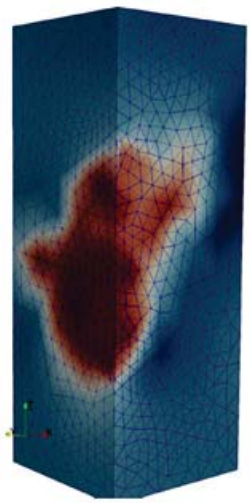
Gianluca Caramiello, Andrea Montanino, Gabriele Della Vecchia and Anna Pandolfi
Dipartimento di Ingegneria Civile ed Ambientale, Politecnico di Milano

Hydraulic fracturing (fracking) is the process of injection of highly pressurized fluid into the soil to create an artificial network of fractures and increase the production of oil and gas reservoirs. Fracking implies different physics: solid mechanics, hydraulics, and fracture mechanics, and the mathematical description of the process is extremely challenging.

The numerical study of fracking has been tackled in the past with oversimplified discrete approaches that disregard the resulting dense network of fractures, require high computational costs, hinder parallelization, and cause unacceptable inaccuracies in the results. By the way of contrast, here we use a continuum material model with microstructures consisting of nested families of equi-spaced cohesive-frictional faults embedded in an elastic matrix. Formation and evolution of the faults are obtained from the minimization of an incremental work of deformation under the conditions of impenetrability of faults and irreversibility of fractures.

The process is governed by the coupled equations of porous media, where the unknowns are displacements and fluid pressures. The problem is discretized in finite elements and solved using a partitioned approach: the equilibrium equations, highly non-linear and history dependent, are solved explicitly; the continuity equation is solved implicitly.

The code, developed during the LISA project HYPER, requires the demanding solution of a minimization problem at each integration point of the mesh and at each time step. The local minimization, the large scale of the computational domain, the reduced stable time steps, and the duration of the fracking process ask for parallelization. The code has been parallelized with shared memory algorithms and used in the clusters of Cineca for running simulations in acceptable times.



Fracking job at a laboratory scale: Simulated damaged zone.

A large number of analyses (160.000 cpu h) were devoted to model fracking processes at the reservoir scale, to assess the effectiveness of different operational parameters, see Fig. 1. The results have been finalized in a scientific publication (G. Caramiello, A. Montanino, G. Della Vecchia, and A. Pandolfi. An approach to hydraulic fracture in geomaterials through a porous brittle damage material model. Advanced Modeling and Simulation in Engineering Sciences, 5(1), 23, 2018.)

Acknowledgment
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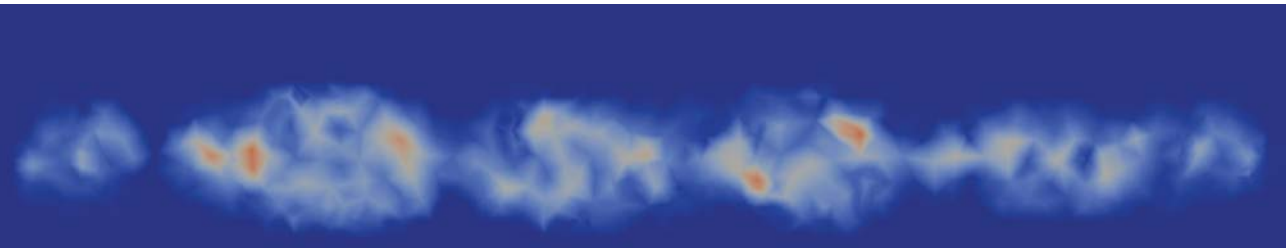

Extension of the damaged zone at a reservoir scale.

High fidelity simulation of nasal airflow patterns in the healthy nose

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Alberto Maria Saibene **ASST Santi Paolo e Carlo, Milano**

During the last years Computational Fluid Dynamics (CFD) has proven a valuable tool for studying the nasal airflow patterns. However, no matter how promising, clinical relevance is further hindered by the complete lack of data on what a normal/efficient nasal airflow should be and what the surgeons should do in order to improve it. Our ongoing interdisciplinary effort within the established OpenNOSE project, joint with M.Quadrio at the Aerospace Sciences and Technologies Department of the Politecnico di Milano, has partly overcome these limitations by the introduction of highly advanced simulations, able to pave the way to a clinical use of CFD in ENT practice.

Many studies have been performed in nasal cavity geometries, however few are the studies employing the LES or DNS approach and mostly consider only simplified or idealized anatomies.

The main objective of this proposal was the creation of a large high-fidelity (DNS and LES) data library for the flow simulations of nasal cavities. A significant number of CT scans of neurosurgical patients has been obtained after the assessment of their nasal function with specific questionnaires (SNOT 22) and the numerical simulation has been carried out.

The proposed CFD procedure from the CT scan to the numerical simulation is completely based on open-source software, and has been developed from our group during the last years [1].

The simulations were performed for both the steady expiration and the inspiration phase mainly by means of the LES technique, for different breathing levels and using computational grid from 2 to 50 million of cells. Furthermore, some acquired CT scan have been used for the simulation of water droplets delivery, coupling the Lagrangian approach with the LES technique.

In the figure streamlines of an instantaneous LES flow field are drawn along the upper region of the cavity w.r.t. a steady inspiration at medium breathing intensity, corresponding to $\Delta p = 20$ Pa, and colored according to the value of the local velocity magnitude with the mucosa lining and the external surface of the face are shown in partial transparency.

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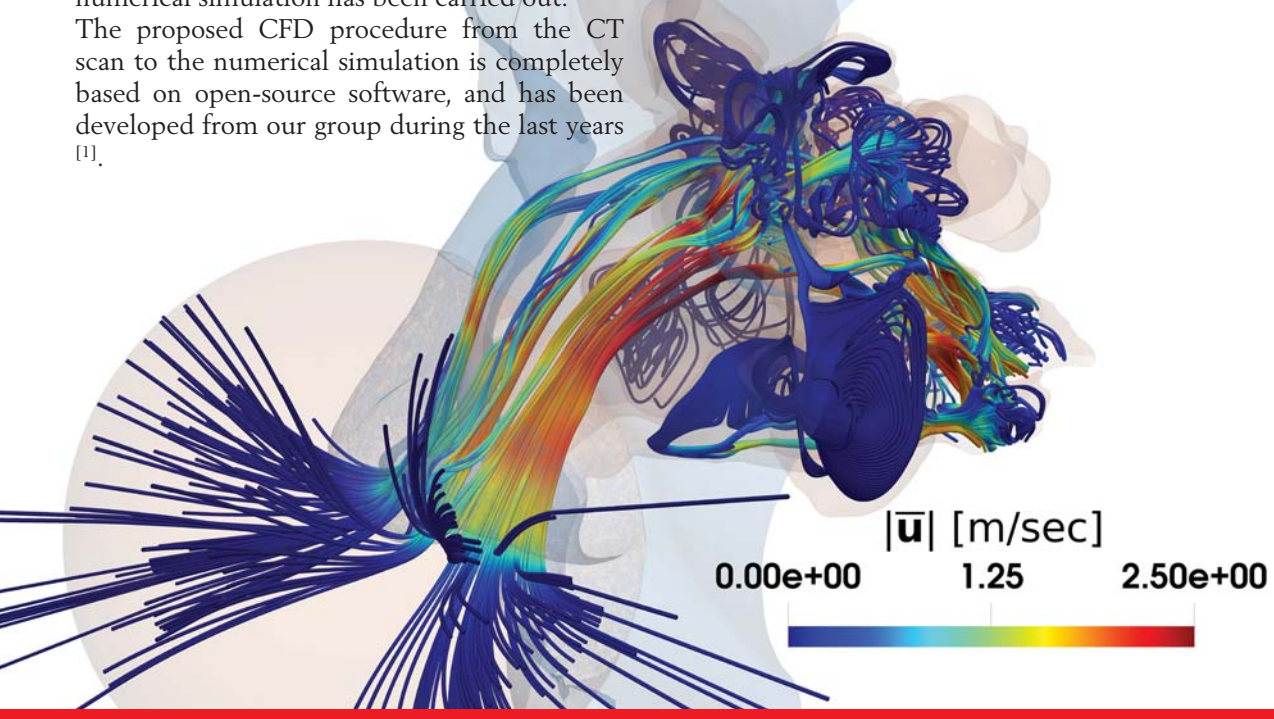
Acknowledgement
We acknowledge the Cineca and the Regione Lombardia award under the LISA initiative 2016-2018, for the availability of high performance computing resources.

Streamlines along the nasal cavity, for $\Delta p = 20$ Pa, colored by the value of the local velocity magnitude.



All-atoms simulations of the spliceosome machinery

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To give life to its end product, a gene must be first copied and then processed to create a filament of mature and functional messenger RNA (mRNA). This latter is responsible for carrying the information contained in the DNA to the other cellular compartments, where it is transformed into proteins. Nevertheless, the messenger RNA, created as a first copy of a gene, is composed by protein-coding regions (exons) and other non-coding regions (introns). To have a mRNA molecule able to transport information usefully, precisely and effectively, the introns must be cleaved, while the exon must be joined together, in a process termed as splicing. This sophisticate snip and stitch process is promoted by a majestic machinery named the spliceosome and composed by dozens of proteins and five filaments of RNAs. Splicing must occur with single nucleotide precisions as its defect is the underlying cause of more than 200 human diseases, including several types of cancer.

A thorough understanding of splicing is pivotal for biology and medicine, holding the promise of harnessing it for genome modulation applications. Recent cryo-EM studies provided an atomic-resolution picture of the spliceosome of different steps of the splicing cycle. Building on the first SPL structure solved at near–atomic-level resolution, Casalino et al [1] performed the first all-atom simulations of the intron lariat spliceosome complex from yeast S. Pombe via multi-microsecond-long molecular-dynamics simulations of ~1,000,000 atoms models. This study elucidated the cooperative motions underlying the functional dynamics of the spliceosome at a late stage of the splicing cycle, suggesting the role of specific proteins involved in the spliceosome disassembly.

In particular, this work assigned to the Spp42 protein the role of an orchestra conductor of a gene maturation symphony by disclosing how it leads the motions of distinct proteins and RNAs assembled in the spliceosome. This study provided evidences for an involvement of Cwf19 protein in the spliceosome disassembly. Hence, his work dispenses a noteworthy piece of knowledge for a thorough mechanistic understanding of this fundamental step of gene expression.

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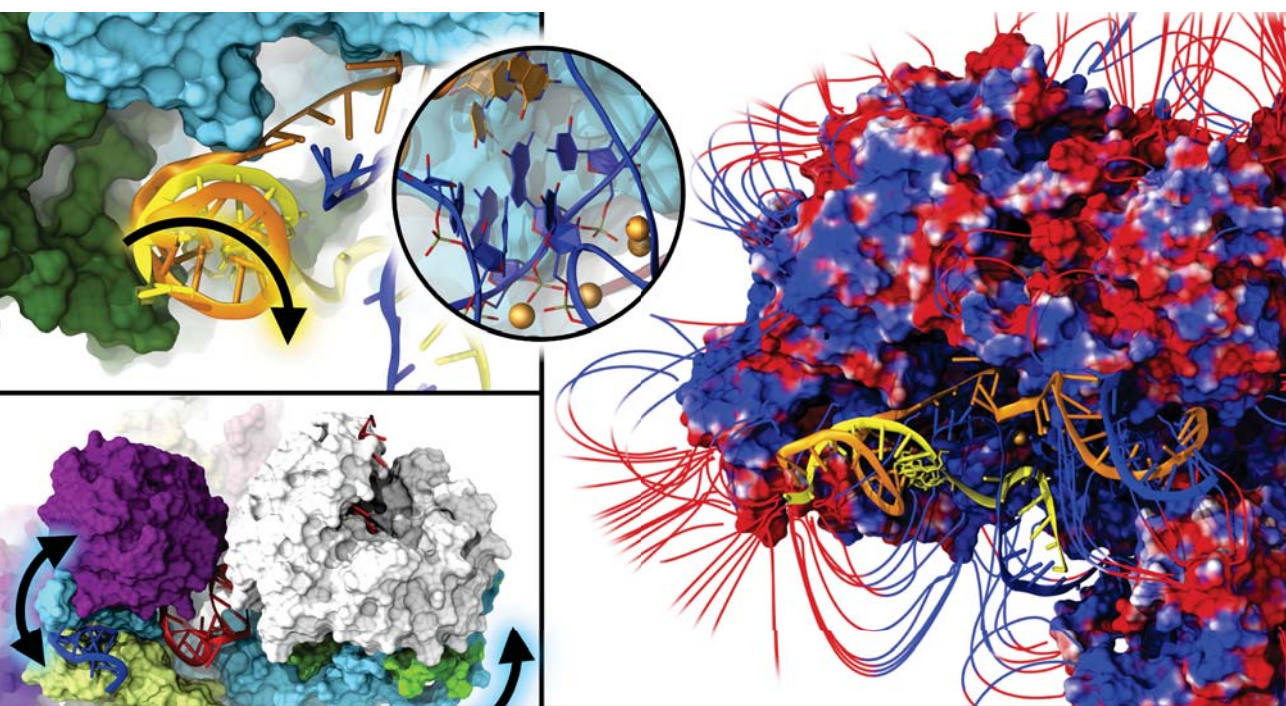
Functional dynamics underlying gene maturation as promoted by the spliceosome. Electrostatic potential of the spliceosome assembly shown in red and blue for the negative and positive regions, respectively, with RNA filaments depicted as yellow, orange and blue ribbons. The Mg2+ ions of the active site are depicted as orange spheres.



Computational engineering for the heart: a multi-physics model for medical support

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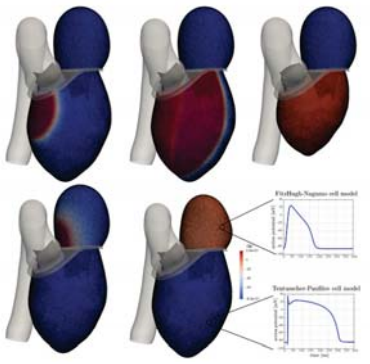
Cardiovascular disorders (CVD) are the leading cause of death in developed countries causing huge economic and societal costs. Overall, CVD cost the EU economy €210 billion per year[1,2] and this expenditure will at least triple by 2050[3]. Progress in medical research has improved the prognoses for CVDs but these advances have now come to a halt[4,5] because of increasing risk factors that are strongly correlated to CVD[6]. Innovative tools are therefore needed for the improvement of treatment outcomes without increasing the medical costs. Computational engineering can provide fundamental contributions in this direction by virtual models capable of adding predicting capabilities to the existing diagnostic tools.

With the above motivations, in this project we have developed a multiphysics model of the left heart that can cope with the electrophysiology of the myocardium, its active contraction, the dynamics of the valves and the complex hemodynamics. The models are coupled with each other thus capturing the fully synergistic physics of the heart.

In our model we have resorted to our massive parallel Navier-Stokes solver AFiD[7], a structure solver based on the interaction potential approach[8], the immersed boundary method with fluid/structure interaction and a bidomain electrophysiology model[9]. The whole package has been parallelized using openMP/MPI directives in order to exploit the computational power of massive parallel architectures. Finally the model has been validated against in-house experiments aimed at replicating one-to-one the computational set-up.

Figure 1: Snapshots of the activation potential during the cycle.



In the figure below we report the dynamics of the contraction and relaxation of the left heart that is triggered by the propagation of the activation electrical. In the same figure we report also the flow streamlines and the wall shear stress at the ventricle during the E-wave of the diastole. The reproduction of all the physiologic heart parameters confirms the reliability of the computational model and we plan to fully exploit its potential by simulating pathologic configurations to support the heart surgeons for the clinical decisions.

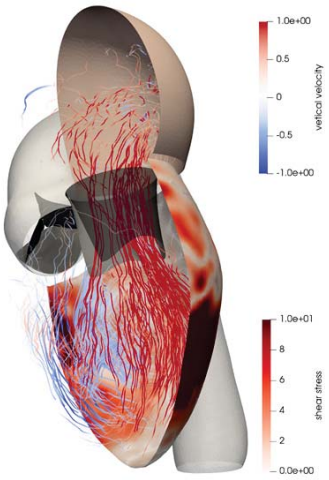


Figure 2: Snapshot of streamlines coloured with the vertical velocity and wall shear stress on the tissue wet surface at the peak of the E-wave of the diastole.

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MD simulations of the effect of different surfactants on the surface tension of a water-oil interface

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The goal is to study the effect of surfactants to immiscible fluid displacement. Surfactants (surface-active-agents) are compounds that lower the surface tension between two liquids or between a liquid and a solid. Surfactants are used in several industries, including enhanced oil recovery from nanoporous rocks, although their effect at this scale is not well understood.
In this project, we develop and study all-atom models for different surfactants (SDS and DTAB) to be used in molecular dynamics simulations with LAMMPS.
To measure the surface tension, we choose the Young-Laplace equation

$$\Delta p = \gamma \left(\frac{1}{R_1} + \frac{1}{R_2} \right)$$

as the most reliable and noise-free method available.
The simulation setup to measure the surface tension, and the effect of surfactants on it, in bulk requires a curved interface to use the Young-Laplace equation. We arrange heptane molecules in a cylindrical shape surrounded by water, or the opposite, and surfactant molecules on the interface.
We run simulations with a water drop in heptane, and with a heptane drop in water. We expect the same surface tension in both cases.
We find that the surface tension decreases linearly with the increase of the surface density of surfactant molecules. The strange behavior of the SDS molecule for low surfactant densities might be due to an imperfect parametrization of the head of the molecule.

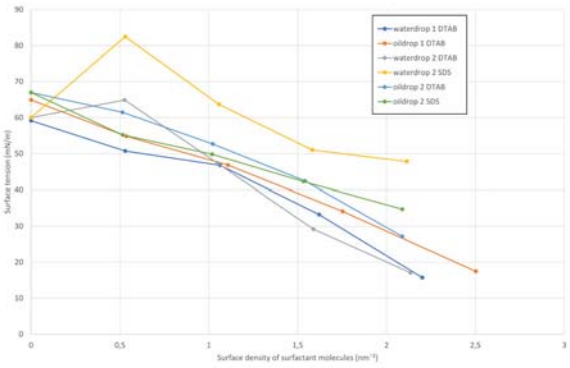

Figure 1: Reduction in surface tension with increasing density of surfactants on the surface, for a water drop in heptane and a heptane drop in water, for different surfactants (DTAB and SDS) and different initial configurations (1 and 2).

The next goal is to study the effect of surfactant molecules in nanoconfinement.
Despite having large error bars, we obtain again a reduction of the surface tension using the Young-Laplace equation.
The surfactants influence the transport properties of water and heptane in a nanotube: the velocities increase with the number of surfactant molecules, compatibly with the reduction in surface tension. Thus, this study gives a scientific background for the common use of surfactants for enhanced oil recovery.

Acknowledgment
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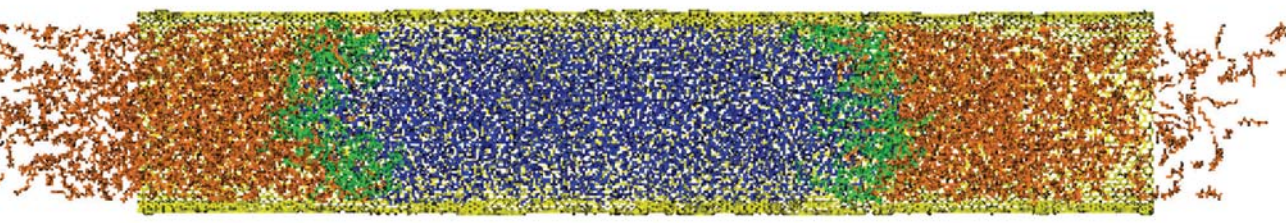

Figure 2: The geometry for confinement. Water is blue, heptane is orange, the DTAB surfactant is green, and the nanotube is yellow.

Magnetic reconnection and turbulence in astrophysical plasmas

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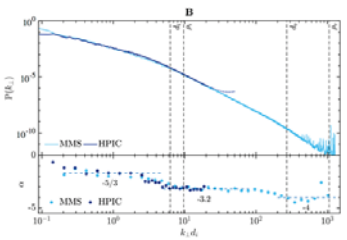
The process of turbulence dissipation in astrophysical plasmas is still unclear and represents one of the great challenges in the field of physics of laboratory, spatial and astrophysical plasmas. The reason is to be found in the nature of the collisions between charged particles and in the fact that in almost all cases we deal with very rarefied and warm plasmas, whereby the dissipation occurs at the scales where the kinetic physics of the single species dominates.

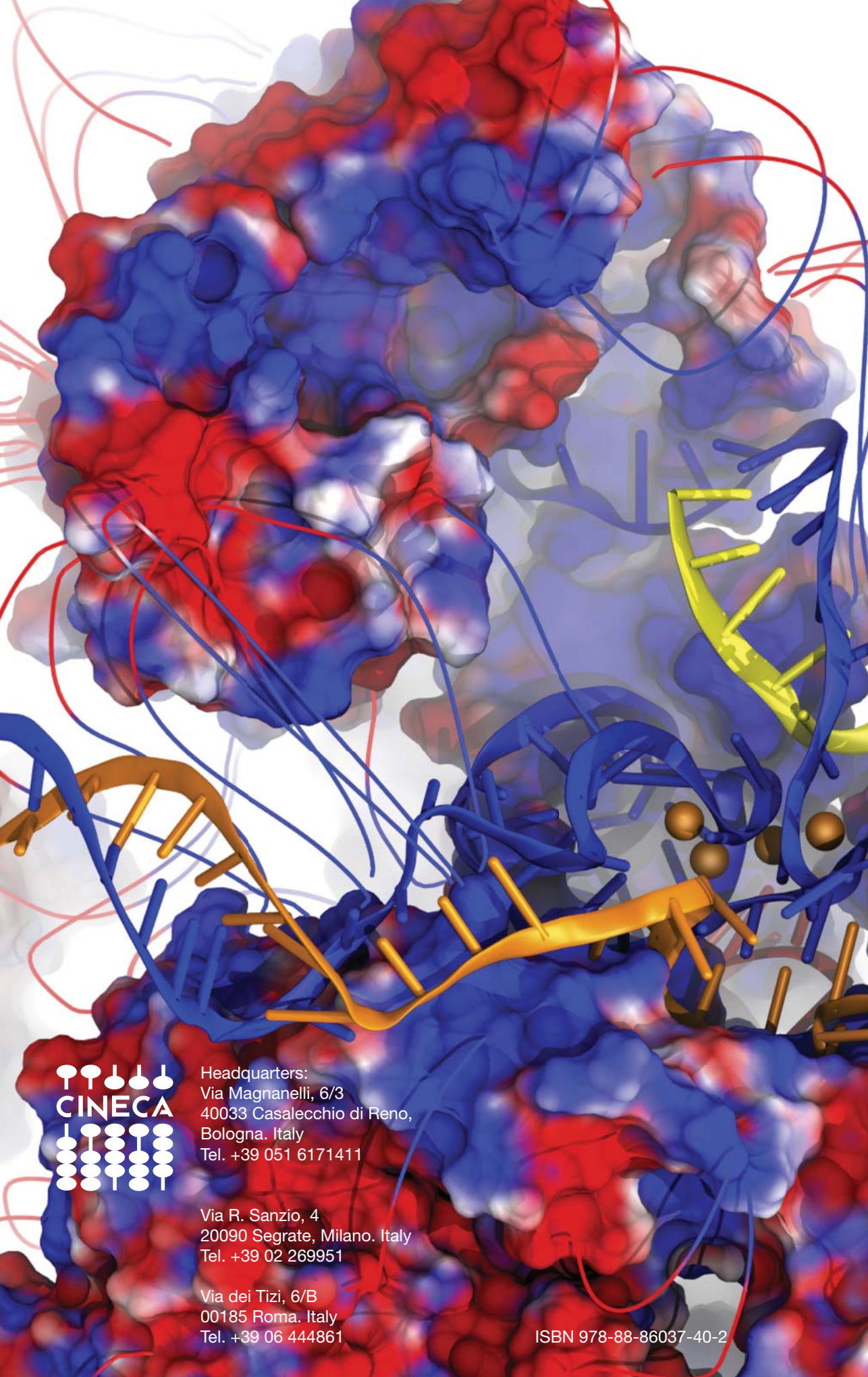
To understand and characterize the transfer of energy from large to small scales, it is essential to use high resolution numerical simulations covering fluid scales (simulations in magneto-fluid regime, or MHD) and characteristic kinetic scales (kinetic simulations) and, where it is possible, for example around the transition region of the turbulent spectrum, to use both fluids and fluid-kinetic hybrids. Such high-resolution simulations, covering a sufficiently large range of scales, allowed to reproduce numerous properties of the turbulent spectrum covering the transition region between the fluid and kinetic regime and being able to follow the evolution of the turbulent cascade during the expansion of supersonic flows.

The most recent high-resolution simulations either fluid or kinetic have shown that a fundamental role in characterizing the process of transferring energy to small scales is played by the process called "magnetic reconnection" where the magnetic field, through a topological transformation, passes from one configuration to another less energetic, with the consequent conversion of its energy into heat. Reconnection is an effective process in extremely localized areas where the presence of strong magnetic field gradients involves the presence of strong currents.

These regions, called current sheets, are continuously formed by the interaction of magnetic vortexes and, if sufficiently intense, can activate the process of magnetic reconnection much faster than the "ideal" evolution of the system, allowing the magnetic energy to dissipate.



Magnetic turbulent eddies in high resolution MHD simulation of decaying turbulence using ECHO (left) and a Comparison between magnetic power spectra measured by the NASA mission MMS in the earth's Magnetosphere with a high resolution simulation using the Hybrid Particle In Cell (HPIC) code CAMELIA. (http://terezka.asu.cas.cz/helinger/camelia.html)



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