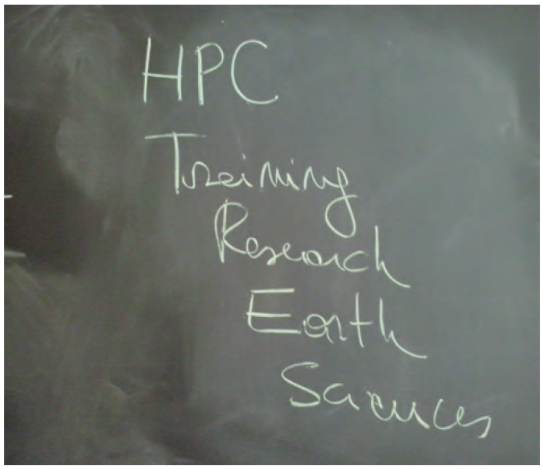
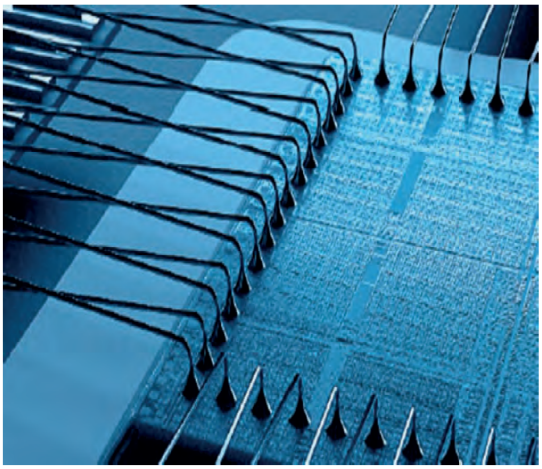
HPCTRES

High Performance Computing





Training and Research for Earth Sciences

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Foreword

OGS (Istituto Nazionale di Oceanografia e di Geofisica Sperimentale - National Institute of Oceanography and Experimental Geophysics) and CINECA drew up an agreement [1] to implement a training program focussed on High Performance Computing (HPC) applications for Earth Sciences, the **"HPC Training and Research for Earth Sciences" (HPC-TRES)**. The program is co-sponsored by the Minister of Education, University and Research (MIUR) under its extraordinary contribute for the Italian participation to activities related to the international infrastructure PRACE – The Partnership for Advanced Computing in Europe[2].

The major objectives of the program are: capacity building, enhancement of human resources, and advanced training in the fields of Earth System modelling (atmosphere, hydrosphere, litosphere and biosphere) and numerical models, the latter considered as a strategic cross-cutting element for modelling activities. These objectives will be pursued through the use of national and European HPC infrastructures and services in the framework of PRACE, the optimization of algorithms and numerical codes, the optimal management of "Earth Sciences Big Data", and the graphical visualization techniques for multidisciplinary applications in the Earth Sciences, also in the frame of the "Blue Growth" strategy.
Therefore, HPC-TRES agreement will establish, sponsor and oversee **training and research awards** (i.e. contributes for training and research activities set up according to current regulations that regulate scholarships – to be also used for masters and specialized courses in HPC -, research grants and PhDs) that will support the research lines **scientific plan**[3] **of the HPC-TRES program**.

Some Italian research groups and institutions (INGV-Pisa, CNR/ISAC, CNR/IGG, CMCC, ICTP-ESP), where the external members of the HPC-TRES Steering Committee lead their research activities and personally contributed to define the scientific plan of the HPC-TRES program, have already subscribed the HPC-TRES initiative, offering logistic support and hospitality to the winners of the training and research awards sponsored by OGS.
OGS recognizes the scientific excellence of the hosting institutions as strategic to the educational and professional growth of the awarded young researchers. OGS is committed to extend the participation to the scientific plan to other national research groups involved in HPC applications for Earth Sciences (2016: MOX-Polimi, ENEA-SSPT, INGV-SST, INGV-CNT, Univ. Bicocca, CRS4; 2017: EURAC, ARPA-FVG; 2018: CIMA; 2019: Univ. Trieste), so that these groups could propose new training and research activities for the next HPC-TRES Calls.

[1] OGS BoD document n. 7.4.2014, date 18/06/2014.

[2] www.prace-ri.eu

[3] The scientific plan was initially written by the HPC-TRES Steering Committee, jointly appointed by OGS and CINECA (OGS BoD document n. 15.9.2014, date 18/12/2014) and composed by scientific experts involved in different HPC applications for Earth Sciences. It is annually updated with new research lines.

Topic A: HPC for Oceanography and Biogeochemistry modelling

Line A1. Biogeochemical forecast skill assessment for Operational Oceanography

In the frame of the European initiatives for Operational Oceanography (e.g. Copernicus Marine Environment Monitoring Services - CMEMS, http://marine.copernicus.eu/), this research line aims at providing numerical tools able to evaluate and improve the reliability and the uncertainty of the operational forecasts produced by coupled physical-biogeochemical models. This activity has important consequences for: 1) support environmental agencies and other stakeholders with useful indications related to the definition of the targets for the Good Environmental Status, as described in the Marine Strategy Framework Directive, and 2) assess the climate projections impacts on the marine biogeochemistry and ecosystems.
Biogeochemical models have different degrees of complexity, and are usually characterized by a high number of parameters: the global sensitivity analysis approach must be based on a large number of independent simulations, such as an ensemble of $O(10^4)$ members, in order to evaluate the model sensitivity to each parameter. HPC can greatly support this activity by widening the ensemble set, initially to assess the model sensitivity (as in the PRACE GSENSMED project), and then to effectively support operational forecast.
Optimization of data assimilation (DA) schemes for the operational biogeochemical modelling constitutes another strategic activity of this research line. Presently, the computational time requested for the convergence of the DA scheme for one single day of analysis is comparable to that one necessary for the completion of a 17-day operational run in the CMEMS workflow for the short-term forecasts of the Mediterranean Sea biogeochemistry.
The multi-platform and multi-variate data assimilation constitutes a state-of-the-art issue of this research line. In the frame of the CMEMS-MASSIMILI project, we are committed to develop a novel DA system to assimilate the data provided by the Mediterranean Bio-Argo floats network into the CMEMS operational model.
Improving of the CMEMS model system performances is significantly related to the capacity of the model to correctly reproduce the interactions of the optical properties with the circulation and the biogeochemical cycles. The development of an optical model that may inherently solve the extinction coefficient as a function of the biogeochemical and physical properties, rather than being externally imposed as a parameter (e.g. from satellite measures), is the goal of this activity. These developments are beneficial not only for the operational oceanography but for the climate studies also, where, in the case of future projections, it is not possible to constrain the model with satellite observations, and the optical properties of the water masses could be simulated by the model as an emergent property.

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Line A2. Evolution of Individual-Based Models towards exascale computing ("Exafish")

Currently most of the biogeochemical and ecosystem models are still based on the assumption that living organisms are homogenously distributed over the volume defining a model domain

cell, as if they were dissolved chemical compounds. In fact, while it is obvious that organisms are discrete entities and should be regarded as such, the use of Individual-Based Models in describing marine biogeochemistry and ecosystem dynamic has been hindered by the intrinsic complexity of the system to be described and the computational load required for comprehensive simulations over realistic spatial domains. The possibility offered by recent HPC developments might give new boost to this field. A challenge is to describe the time evolution of the interaction between different typologies of organisms within a food web, each type being defined by an ensemble of slightly different individuals. A second challenge is to use exascale computing to simulate the spatial-temporal dynamics of the resulting huge number of interacting organisms by means of a Lagrangian approach. A third challenge is the analysis of the huge amount of data provided as model output, possibly also in order to derive ecologically based subgrid parametrization of biogeochemical and ecological processes.

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Line A3. Simulations of behaviours, responses, and adaptive and evolutionary characteristics of marine ecosystems

The goal of this research line is the development of new model paradigms aimed to simulate behaviours, responses, and adaptive/evolutionary characteristics (also referred to as "traits") of the marine ecosystems, with a strong dependency on natural drivers (e.g. increasing of the temperature field) and anthropic pressures (e.g. environment management). These new models will be able to provide more realistic estimates of the effects related both to global long-term climatic changes and to local environmental policies on marine ecosystems and their resources.
To this scope, innovative algorithms will be specifically designed to efficiently exploit the future heterogeneous HPC architectures, as for example a lattice-Boltzmann approach to solve transport equation on 3d meshes of $O(10^8)$ nodes. This activity will request new ad hoc parameterization/discretization developments and innovative programming techniques, binding together technological and scientific challenges and capacity building.
The added value will be constituted by the rise of a new ecological modelling community operating in an unexplored scientific field, able to define new evolutionary schemes never considered before. Therefore, we expect a significant commitment on the training and collaborative basis (e.g. the development of new expertise in computational ecology, the organization of a summer school on new paradigms in ecological modelling, international scientific collaboration).

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Line A4. Parallelization of hydrodynamic finite element models

Hydrodynamic finite element models (FEMs) can be used to perform high-resolution simulations of areas characterized by complex geometry and bathymetry, such as lagoons, estuaries, coastal areas, lakes (though some FEMs are also applied for global ocean

simulations[4]). Such models can be often legacy codes originally written for sequential execution, which appear today significantly limited given the possible applications able to exploit the larger availability of HPC resources.
An application of this research line is the parallelization of the Shallow water Hydrodynamic Finite Element Model (SHYFEM).

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Line A5. New algorithmic approaches for ocean models at exascale

Access to large computational capabilities allows increasing both the resolution and the complexity of ocean models/simulations. However, the efficiency of the current models has to be improved. One of the main limits is the low scalability of legacy codes on many core architectures, usually compromised by the data movement intended at different levels, such as communication, memory access, I/O, etc.
The research line aims at the re-design at algorithmic level of target ocean numerical models through the following steps: (a) definition of the main bottlenecks to the efficiency of parallel codes and the exploitation of the peak performance of the new generation HPC systems (b) investigation of algorithms and innovative architecture-oriented technologies for the optimisation and parallelization of numerical simulation codes and (c) exploration of new opportunities, such as Hybrid Numerical Models (HNMs), based on combining deterministic modeling and machine learning components.

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Line A6. Multi-component operational modelling systems for Regional Environmental Protection

Numerical modeling plays a key role in supporting the activities of the Regional Environmental Protection Agency of Friuli Venezia Giulia (ARPA FVG), providing quantitative cause-effect relationships within the DPSIR conceptual framework (Driving forces, Pressures, State, Impacts, Responses). ARPA FVG already manages operational modeling chains, based on the some numerical models running on the regional HPC facility (http://gridfvg.e-science.it/) such as WRF (for mesoscale numerical weather prediction system), FARM (for air quality forecast and assessment), SPRAY (for airborne pollutant dispersion at meso and microscale) and INEMAR (for regional Atmosphere Emissions Inventory). Further, many of ARPA functions deal with marine and coastal environment monitoring and management, whose area of interest includes the Gulf of Trieste and the Marano-Grado Lagoon.

[4] e.g. FEOM, see http://www.awi.de/en/research/research_divisions/climate_science/climate_dynamics/methods/finite_element_ocean_model_feom/

Some specific needs have been identified, requiring an integrated, multi-component modeling system to be gradually assembled and set up in operational mode. In particular, short-term operational products (thermohaline fields and currents forecasts at ~5 days, both in Gulf of Trieste at ~1 km resolution and in Marano-Grado Lagoon at ~0.1 km resolution), medium-term operational products: solar penetration, oxygen and chlorophyll concentration forecasts (same requirements as above), long-term operational and non-operational products. The latter are strategic both for sea (oil spill trajectory forecasting, forecasts and back-trajectories of transport of floating marine debris, forecast, assessment and scenarios of pollutants and nutrients dispersion from marine outfalls, forecast, assessment and scenarios of diffusion of pollutants carried by Tagliamento –microbiological- and Isonzo –mercury- rivers) and for the lagoon (assessment and scenarios of sediment transport and lagoon morphology).
Even if models and methods are already available and well assessed for each of the topics considered in the project, still some scientific and technological challenging efforts can be easily foreseen in the operational requirements for the modeling systems and in data collection, organization and management (in particular dealing with pollution sources and freshwater/groundwater inflows).
This research line should benefit from results expected from Line A4, "Parallelization of hydrodynamic finite element models".

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Line A7. Numerical models for sound propagation in stratified water basins

The propagation of an acoustic signal in a non-uniform field is a subject of paramount importance, given the growing and uncontrolled noise pollution present in the oceans, which has been reported for years by the scientific community, as a cause of severe discomfort against many underwater animal species.
The characterization of the noise source may be reproduced very accurately using Large Eddy simulations, coupled with the Ffowcs Williams and Hawkings model. The first reproduces in detail the noise sources: among the others, airguns for geological intrusive explorations, the wake of a propeller or the implosion of a cloud of cavitation bubbles. The acoustic model acts as a post processor on dynamic fluid data; it provides a time dependent pressure signal in specific points in space. The weak point of this approach, which appears as the state of the art in hydroacoustics and has become coveted by most shipbuilding companies, is that it assumes a uniform medium.
This assumption is somewhat oversimplified, since the underwater environment is by far not uniform, meaning that the water density changes in space due to variation of temperature and salinity along the water column. This causes the variation in space of the speed of sound. Also, the bottom and the free surface cause relevant effects of reflection and refraction. Idealized studies of the propagation of sound emitted by point sources in a stratified environment are present in recent literature.
In the present research line, the analysis will be extended to the more interesting case of more complex noise sources as those mentioned above. Specifically, the tailed characterization of the acoustic source and its propagation in stratified environments. The software used is an open source software, named OpenFoam, and it is suitable for modifications and additions of new modules. Tests and possible validations of the developed model can be based on cases of practical interest, such as ship propellers and airguns. The study will be carried out numerically, taking advantage of high performance computational platforms. In fact the

problem under investigation will require the use of unsteady massive parallel-architecture simulations over grid topologies composed of 108-109 grid cells. Also, the parallelization of the acoustic solver will certainly be performed, in order to optimize the computational process.

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Line A8. Study of the evolution of chlorophyll fronts through high resolution models, HF radars and data assimilation

To assess the impact of anthropogenic pollutants on marine and coastal ecosystems (including HNS, plastic marine litter, organic micropollutants, etc.) a large number of multi-disciplinary skills and tools is needed, such as observation systems (in-situ and satellite) and numerical models. Numerical models are fundamental tools to get a three-dimensional description of the main physical and biogeochemical processes, both to analyze past situations supported by observations, and to make predictions. Although models suffer from uncertainties that need to be reduced to make more accurate assessments, their support is essential in several fields. As an example, the space-time evolution of productive oceanic features (chlorophyll-a fronts), strictly depending on oceanographic flow field, is necessary to study the feeding habitat of a number of marine species. Satellites with low revisit time provide valuable observations of chlorophyll fronts but are not sufficient to characterize its subsurface structure. On the other hand, the modelling of the trajectory of pollutants of punctual and widespread origin, may suffer from the uncertainties affecting the hydrodynamic models output. Therefore, we consider necessary: 1) to increase the resolution of the numerical models in use, to allow the representation of fundamental physical and biogeochemical features for ecosystem assessments, currently not well described in most of the (operational) models in use; 2) to reduce the uncertainty of such models through data assimilation. The realization of such a model necessarily requires the support of high-performance computational tools.
The proposed activity will implement a combined physical-biogeochemical model in the North-Western Mediterranean area including the PELAGOS Sanctuary (a Specially Protected Areas of Mediterranean Importance). The area is of great importance both for the occurrence of significant oceanographic processes (including the development of the North Mediterranean current and deep water formation), and for the remarkable presence of marine mammals suffering from numerous threatening factors (ingestion of plastic marine litter and hydrocarbons). It is then important to rely on accurate numerical models to identify feeding habitats of cetaceans and assess the risks associated with the potential compresence of pollutants.
The benefits associated with the assimilation of data on a regional scale model will be assessed comparing the results from the use of already available models. Observations will include satellite data (available through CMEMS) and additional data coming from the HF radar network present in the North-Western Mediterranean, and made available through SICOMAR , IMPACT, SICOMARplus and SHAREMED projects.
In the first part the activity involves the implementation of models and procedures for reducing uncertainties. In the second part, the evolution of chlorophyll fronts will be analyzed. Comparisons between model outputs and satellite data will be carried out, together with the

results of feeding habitat models and cetacean sightings, available through the GIAS project, and in collaboration with other entities operating in the PELAGOS Sanctuary.

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Topic B: HPC for Solid Earth modelling

Line B1. Numerical simulation of earthquake ground motion in three-dimensional models of the Earth's crust

Numerical simulations of earthquake scenarios based on the solution of the wave equation in three-dimensional viscoelastic heterogeneous media represent a promising tool for the studies of seismic hazard aimed at the mitigation of the seismic risk but they can be performed only with HPC resources.
In order to perform these simulations, our research group developed the parallel code FPSM3D (Klin et al. 2010), based on the method for the solution of differential equations known as " Fourier pseudospectral method". The accuracy of the method and the code was recently confirmed with the participation of our group to a comparative exercise of numerical simulations of ground motion generated by earthquakes in sedimentary basins (Chaljub et al., in press.). The parallelization of the code uses a hybrid scheme based on the two protocols MPI and OpenMP and is constantly updated with improvements in computational efficiency and in the complexity of the physical model to be treated. With the current implementation of FPSM3D on the supercomputer IBM BG/Q "Fermi" at CINECA a typical simulation requires a computational cost of the order of tens of thousands of core hours and several tens of simulations are needed in order to build up an earthquake scenario. Currently we plan an extensive application of numerical simulations for earthquake scenarios in the Po Valley (Italy).
Innovative versions of code suitable for simulating seismic wave propagation in stochastic media 3D are also under investigation.

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Line B2. Microseismicity data processing

The goal of the project consists in the implementation and testing of a procedure that takes advantage of HPC resources for the automatic detection and location of microseismic events with a local network of receivers in a noisy environment. The use of automated procedures for the detection and location of microseismic events is essential, because of their high number. However microseismic signals are generally characterized by a very low signal to noise ratio that affects the performance of automated standard procedures. Several alternative approaches have been proposed in recent years, among which the most promising consist in the calculation of the probability distribution over a discretized parameter space. HPC techniques are neccesary in order to apply efficiently these methods.
Our research group manages the seismic network of Collalto, an infrastructure aimed at monitoring the natural and induced seismicity in the field of natural gas storage called "Collalto Storage" near Treviso (http://rete-collalto.crs. inogs.it). With the methods under implementation we aim to alleviate the limitations due to the overlap of environmental noise on the recorded signals, to lower the magnitude of completeness and to allow a moment tensor inversion in order to make possible studies that discriminate between natural and induced seismicity. These studies are of increasing interest because of the growing perception of the risk associated with exploitation of earth resources.

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Line B3. Seismic Laboratory set-up (SEISLAB)

The simulation of waves' propagation in complex media is a key activity of the Seismic Laboratory at OGS (SeisLab), used to study rock properties and building 3D models of the Earth. Its applications include energy resources (both hydrocarbon and geothermal), fresh water catchment, CO2 sequestration, seismic hazard, civil engineering and mineral resources in general. High-resolution Earth models, however, require massive calculations, which can be carried out only by parallel, high-performance computing. A toolbox is being developed that allows non-specialist, but computer-literate users, to run high quality simulations of wave propagation to solve geological problems. A goal of the planned work is to add new tools and integrate them in the existing framework, allowing other researchers and students to use them in specific applications.
One of the leading-edge technologies being addressed is the full-waveform inversion. A few elements of this method are available, as numerical modeling techniques, while others need further developments. One of these is a multi-dimensional optimization solver for highly non-linear object functions, where the parameter number may reach many millions, with constraints that may be both relative and absolute. For example, a rock may have a known range of properties from laboratory measurements (absolute constraint) and a maximum change with respect to nearby formations (relative constraint), if the related geological model suggests so. As the related simulations are computationally very expensive, an optimal minimization strategy can provide a major reduction of the computing costs. Methods as the "Pattern Search" are envisaged to be adopted and optimized, in addition to genetic algorithms and possibly newly created approaches.

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Line B4. High level hybrid programming code for geodynamic simulations

The deformation of Earth surface is the result of several forces that act inside the planet: complex models based on theoretic numerical simulations are needed to understand how the Earth surface evolves.
Starting from well-known numerical methodology already used among the geodynamic scientific community, a new software suite PyGmod (Python Geodynamic Modeling) has been developed in the last year. Unlike common simulation code written in Fortran or C the programs of this suite are pure Python for more than 90%, implementing a parallel schema that takes advantage of the new architecture of the last HPC machines. As the most recent HPC facilities are characterized by a distributed shared memory architecture, the code uses standard MPI coupled with a multi-threading parallelization algorithm to speed up some critical (atomic) parts that can benefit of it. Since the OpenMP A.P.I. is not directly accessible by Python, the threading system has been developed with Cython. A real time visualization library, mainly based on Matplotlib, has been developed to inspect results during the computation.
The application simulates large-scale geodynamic processes involving the interaction of tectonic plates, the generation of magma, surface topography evolution, mineral phase changes, etc. The code will be mainly used to understand the dynamic of continental rifting.

Tests have been already done on multi-core machine in house and are now going live on some HPC facilities (GALILEO) provided by CINECA in the ISCRA PYGEO project.

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Line B5. Multiphase flow modelling of explosive eruption dynamics

This research activity focuses on the atmospheric dispersal of the products of explosive activity, namely volcanic gases and pyroclasts, i.e., dispersed particles produced by the fragmentation of the liquid magma in the volcanic conduit. To describe the interaction between the eruptive mixture constituents, this research has been primarily carried out by means of the three-dimensional Eulerian-Eulerian multiphase flow models (describing gas and individual particle classes as interpenetrating and interacting fluids) and equilibrum-Eulerian models, with potential new applications focusing on Eulerian-Lagrangian modelling.
HPC research will be aimed at the understanding of specific multiphase flow processes whose features are still mostly unknown, and specifically: gas-particle turbulence and its control on the dynamics of volcanic plumes; the role of supersonic regimes and shock waves generated during explosive phenomena; the dynamics of particle and velocity stratification in pyroclastic density currents.

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Line B6. Non-equilibrium dynamics in magmatic systems

The unpredictable evolution of volcanic unrest crises is strongly dependent on the complex, non-linear dynamics of magma storage and plumbing systems. Non-equilibrium multiphase flow models are required to describe the interactions among liquid magma, solid crystal phases and exsolved volatiles, which ultimately determine the eruptive potential.
HPC research will aim at the implementation of a three-phase solver within the OpenFOAM framework, capable of handling the specific thermodynamical and rheological equations that characterize magmatic mixtures. The mathematical formulation and the modular, object-oriented numerical implementation will allow to easily include the different constitutive terms, such as viscosity, solubility, crystallization and diffusion models, to quantify their impact on the overall system evolution.
The method of moments will be used to describe the space-time evolution of crystals and bubbles populations in terms of the moments of their respective distribution functions, without the need to retain the microscale details. This will provide a very efficient way to deal with the very different length and time scales that characterize magma dynamics at depth.

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Line B7. Environmental impact of explosive volcanic eruptions and volcanic hazard

The assessment of explosive volcanic hazards (mainly associated to ash fallout from convective plumes and catastrophic pyroclastic density currents) requires a methodology to take into account the high level of uncertainty in initial and boundary conditions, the limited knowledge of the physics of volcanic phenomena and the limitations associated to numerical resolution. Coupling deterministic models (such as PDAC, Vol-CALPUFF and OpenFOAM) with statistical analysis tools (such as DAKOTA) has demonstrated to be effective for simple scalar models. However, coupling of complex 3D parallel models would require a careful code and workflow design, data assimilation, control of load balancing and appropriate sampling of the parameter space to reduce the computational cost of probabilistic analysis.
New HPC applications will focus on: inversion of observation data (such as thermal infrared and visible images of volcanic plumes); coupling between atmospheric and three-dimensional ash dispersal models; ensemble simulation of eruptive scenarios.

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Line B8. Detection of slow slip transients before strong earthquakes

Many strong earthquakes are preceded by one or more foreshocks, but it is unclear how these foreshocks relate to the nucleation process of the mainshock. Laboratory and theoretical studies have proposed that earthquakes are preceded by a nucleation process where stable, slow rupture growth develops into unstable, high-speed rupture within a confined zone on a fault. The devastating earthquake that struck Japan in early 2011 was apparently preceded by small, repeating quakes that migrated slowly to where the disaster took place. Slow slip at the base of the crust was observed also for the 1999 Mw 7.6 Izmit (Turkey) earthquake. If this kind of premonitory slow slip behavior also precedes other strong earthquakes, its knowledge should have critical implications for earthquake prediction and risk assessment. It is therefore essential to inspect thoroughly seismic records of other well-recorded earthquakes in search of similar nucleation processes. Here, we plan to study the seismicity and possible slow slip events related to the last relevant earthquakes that struck Italy. To detect the presence of possible slow slip events would be of fundamental importance to understand whether or not the seismic sequence is a precursor of strong earthquakes. Our study will try to confirm the role of the slow slip transients as possible precursor of strong events. Results will impact on operationally qualified, regularly updated seismicity forecasting systems able to provide advisories to the public and authorities in terms of short-term probabilities of future strong earthquakes.
HPC resources are needed to perform efficiently cross-correlations of daily continuous seismic waveforms for a large number of recording channels and reference "template earthquakes". The testing phase, for some specific strong earthquake, requires to apply the method in retrospect, including months of recorded data before the main event. Distributed calculations allow to exploit a flexible approach to signal time windows, frequency bands, cross correlation thresholds, and other parameters controlling the overall flux and specific parameters of the complex seismic sequences before the strong earthquakes.

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Line B9. Fast GPU-based tsunami simulations and its application to Probabilistic Tsunami Hazard and Forecast

Tsunami wave simulation is characterized by a wide range of spatial scales (from a few meters to thousands of kilometres), typically with time steps on the order of seconds over a simulation that can span several tens of hours. A typical single event tsunami scenario simulation can be normally conducted on a laptop within a time frame of a few hours; however, several factors can significantly increase the computational requirements in tsunami simulations. Firstly, the computational requirements can be increased largely by both the size of the domain or the spatio-temporal resolution. Secondly, the computational requirements are also increased due to the huge number (sometimes as much as tenths of millions) of simulations needed to explore the uncertainties in the tsunamigenic source variability, producing, at the same time, a massive output of data, for example in probabilistic tsunami hazard. In this sense, I/O, pre- and post-processing operations and analyses can also be regarded as a big-data problem. Finally, large computational efforts are necessary to enable real-time tsunami simulations (e.g. for early-warning purposes), for instance towards facilitating local high-resolution inundation simulations before an event strikes. All these reasons make tsunami modelling one of the most challenging scientific areas for HPC nowadays, particularly in the field of GPU computing where recent code developments revealed very promising (e.g. HySEA tsunami simulator).

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Line B10. Imaging and numerical geophysics

The activity is focused on the development and use of mathematical models and advanced information technologies for designing and producing industrial HPC applications for exploration geophysics.
In just a few decades, exploration geophysics has enormously enhanced the capacity to identify and exploit natural resources. The introduction of surveying techniques and high resolution numerical reconstruction have enabled prospectors to see through the earth and develop a clearer understanding of its structure, going well beyond empirical good sense. Such developments in prospecting technology have led to an explosive growth in the field of imaging science.
In seismic imaging, the topic of the present research line, transitioning compute-intensive applications from prototype to industry-ready production software for high-end local clusters of thousands of compute elements is a significant undertaking. Computational complexity must be organized on the available architecture, optimizing parallelization and data movement strategies (mpi, peer-to-peer, thread-based), while taking into account the granularity of the computational infrastructure (fiber, nodes, cores, file systems) and avoiding competition in accessing the resources. Reliability, fault tolerance and recovery mechanisms are topics of special concern in HPC software design for data imaging, especially when the processing of a single job may require several weeks even on powerful supercomputers.
Altogether, this know-how makes the difference between a research prototype and a stable HPC product devised for breakthrough science and industrial production. The project will be

concentrated on the development of a 3D elastic reverse-time-migration (eRTM) application for the concurrent processing of very large volumes of seismic data.

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Line B11. Geologic structure of Italian seas and near land areas by inversion and forward modeling of geophysical data

During the last forty years several geophysical data such as gravity and magnetic has been recorded by OGS in Italy over land and sea areas. These records are fuzzy, not uniform and corrected according to old and sometime different methods. OGS wants to recover all the data, organizes them in a coherent and usable database. This new dataset will be used to do a 3D gravity inversion and thermo-mechanical modeling of the lithosphere in some key areas: the Northern Adriatic Sea, the Friuli Plan, the Sicily Channel and the Southern Ionian Sea. The research activities are organized in three main steps:

1. Collection of every gravity data recorded by OGS from 1965 and apply new correction methodologies. The coupling of old data with Satellite derived ones will improve accuracy and will reduce some gaps in the data coverage. If some areas will show a poor coverage new gravity surveys will be planned. The new dataset will be managed and stored in a GIS database.
2. The new gravity dataset will be used to do a 3D gravity inversion with the parallel software GRAV3D (https://grav3d.readthedocs.io/en/v6.0/). The inversion is solved as an optimization problem with the simultaneous goals of: minimizing a model objective function; generating synthetic data that match observations to within a degree of misfit consistent with the statistics of those data. This software is suitable for large problems since it implements a Message Passing Interface (MPI) interface and is able to take advantage of multi CPU computer for the inversion. Existing seismic and tomographic data will aid the forward inversion in the studied areas. The gravity modeling will provide a detailed picture of the density structure of the lithosphere.
3. The density distribution in the lithosphere is the key to understand the vertical and horizontal movement/adjustment of the lithosphere (isostasy). The shape and geometry of lithological layer inside the lithosphere reflects its thermo-mechanical state. How the lithosphere behaves depends on its rheological stratification, temperature distribution, vertical and horizontal stresses. The lithosphere geometry can be modeled by solving the 3D flexural equation and fit the calculated surface to those extracted by the forward gravity inversion. Furthermore, if the flexural modeling is coupled by the seismic, tomographic data and stratigraphic data a backstripping and reconstruction of the isostatic movements of the area can be achieved. This method is tedious and time consuming since it needs the calculation of several solutions of the 3d flexural equation changing several parameters. The use of and MPI based algorithm can speed up the computation since several solutions can be calculated at the same time. All the software needed for the calculation has been developed by OGS. The parallel code is written in Python, some other utilities are written in Matlab and Python.

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Line B12. Calculation of Damage maps for seismic scenarios in Friuli-Venezia Giulia

Seismic damage maps are extremely helpful for the emergency management in active seismic areas. However, due to the relatively scarce seismic activity in the last decades, there are few examples of risk assessment for the Friuli-Venezia Giulia region, mostly based on macroseismic Intensity seismic hazard assessment and vulnerability matrices (Bernardini et al., 2008; Meroni et al., 2008).
We aim at producing damage maps for two hypothetic scenarios based on the recent revision of the N-E Italy main seismotectonic zones (Bressan et al., 2018). We will develop, test and apply a procedure (based on ground motion forecasting) that can be useful for quasi-real-time calculations of scenario-induced losses, as required for Civil Protection purposes. In order to account for the uncertainty in defining the parameters to be adopted in the scenarios calculations (e.g. seismic source parameters, GMPES, exposures model and fragility curves), we propose to adopt a Monte Carlo approach to initialize each run with a sampled set of parameters. The resulting set of damage/loss distribution will provide a more comprehensive picture of the expected event impact. Calculations will be performed with the OpenQuake program (Silva et al., 2012). In order to increase the usability of results, we will produce different graphic formats (ex. maps, videos, interactive plots) that grasp the complexity of results, yet in a clear way. Such products could support authorities and actors involved in medium and long-term planning in the selection of risk reduction measures and their priorities.

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Line B13. Improving the understanding of site-city interactions for better earthquake risk mitigation

Since earthquakes can neither be prevented nor predicted, improving the planning of urban areas is an important issue to reduce damage to built environment and human losses in the long term. Planning of urban areas may be significantly improved if the variability of ground shaking over short distances that is known to occur during earthquakes is taken into account. When an earthquake occurs, besides the alterations of waves in the shallow geological layers, the interactions between single buildings and the soil might also contribute to modification of ground shaking, and thus, to seismic risk. In urban areas, these interactions are not limited to interactions between single buildings and the soil, but include interactions of an entire city and the soil. Since these interactions are not understood in detail as yet, they are not taken into account in the planning of urban areas and seismic risk assessment and mitigation. Until now, most studies on these effects have been carried out by numerical simulations without the possibility of a comparison between the predicted and the observed seismic wave field. Only a very limited number of analyses tried to tackle the problem based on empirical data sets.
The project aims at improving our understanding of interactions taking place between buildings and the soil and among buildings through the soil during earthquake shaking by using both a unique empirical data set and numerical modeling. Better understanding of the interactions between buildings and the soil may contribute in the long term to identify areas of higher seismic risk and thus, to a better preparedness in case of an earthquake. Furthermore, this knowledge could be included in guidelines for standard risk assessment

and mitigation approaches in urban areas. Finally, improving urban planning in the long term by taking SSI and SCI effects into account, can contribute to reduction of seismic risk.

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Line B14. Imaging and modeling of river banks and levees

River banks and levees are continuously subjected to natural events (animal activity, flow erosion, floods, ...). Thus, these structures represent dynamical systems that can know drastic - and even catastrophic - changes.
In Italy, the need to evaluate, monitor and anticipate the risks related to these structures has led to many monitoring and measuring campaigns by several companies and institutes for the last decades. However, the scope of each of these campaigns was usually very local, and the techniques employed were very diverse (from historical logs and visual observation to both geotechnical and geophysical measurements). Carrying the effort to build a large scale model and methodology to study and consolidate efficiently the structure of river banks and levees, the DILEMMA project involves 3 multidisciplinary entities (POLIMI, OGS, and UNIPR), each having their own set of competences.
In order to accurately model the structure and behavior of river banks, geotechnical parameters have to be extracted from physical measurements (EM, GPR, DUALEM). Using geotechnical and/or geophysical methods (and combinations thereof), relevant parameters can be inverted from the measured data. These inversion methods require the proper modeling of the associated forward problem for each method, namely: being able to reproduce the measured data with synthetic records. Solving for either the forward problem or the inverse problem can prove computationally intensive, even in an HPC environment.
OGS participates to the DILEMMA project by lending both its expertise and experience in the development and optimization of numerical modeling codes for geophysical applications in an HPC environment.

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Line B15. GNSS data processing

The aim of the project is the implementation of a system for fast and reliable GNSS data elaboration. GNSS is a complex system of satellites that involves the well-known GPS and other constellations such GLONASS or the more recent Galileo and Beidou. GNSS is utilized to provide the position of a GNSS sensor, also called Continuously Operating Reference Station (CORS), deployed on the region of interest. Position time series and derived velocity fields can be employed, after a devoted elaboration process, for crustal deformation studies as a support for the seismology researches.
Our group manages the GNSS CORS network (16 sites) called FReDNet which has been projected to monitor crustal deformation along northeast boundary of the Adriatic microplate in the Friuli-Venezia Giulia region (more information at http://frednet.crs.inogs.it). To increase the measuring point density and the velocity field quality, different CORS must be added to the FReDNet frame data analysis. Furthermore, in order to produce robust final velocity estimates, several software can be taken into consideration, we want to focus our proposal into the comparison between two of them which use different approaches to solve

the problem: GAMIT/GLOBK (http://geoweb.mit.edu/gg/) developed by MIT Scripps Institution of Oceanography and Harvard University and GPSY (https://gipsy-oasis.jpl.nasa.gov/) developed by the Jet Propulsion Laboratory (JPL).
In the last two years, we have used the MARCONI platform to test the GAMIT/GLOBK features and compatibility with the HPC resources. We think that HPC capacities are crucial to elaborate decades of data logged by hundreds of stations deployed in, and near, the Italian North-east area (our region of interest and site of the 1976 earthquake). Furthermore, we believe HPC resources will represents the best approach to robustly evaluate the GNSS velocity field in a short time. As and added value, our GNSS data and products are included inside an agreement to support the Joint Research Unit (JRU) EPOS-Italy: a national JRU to sustain the European Plate Observing System project EPOS (see at: https://www.epos-ip.org/). The yielded products will advertise the solution found with the help of HPC and will turn on the GNSS community interest at European level. Finally, as further advantage, our software tests and elaborations can be used to deploy stable packages on the HPC resources and available, as a standard module, for other research teams. The solution will speed up greatly the analysis for the GNSS community and will ensure a reliable and robust access to the whole analysis process.

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Topic C: HPC for Earth System modelling

Line C1. High-resolution simulations of convective processes in the Earth System

Convection is an essential process in the Earth System, transporting heat and material in the atmosphere, the oceans, subsurface aquifers and the Earth mantle. At the same time, convective processes represent a paradigmatic example whose study has led to the development of many new ideas on the nonlinear dynamics of complex systems. The simulation and analysis of convective processes requires sophisticated simulation methods and powerful computing resources, to resolve the many scales at work. This research project is devoted to the development and implementation of numerical methods for high-resolution simulation of convective processes in the Earth System.
Research activities will include a first part devoted to simulating convection in idealized configurations, and a subsequent phase dealing with the application to a specific geophysical setting (atmosphere, ocean, or subsurface flows), to be defined based on the background of the fellowship recipient and the research priorities. From a technical viewpoint, this line aims to contribute to the development and improvement of numerical codes for convection simulations. From a scientific viewpoint, the research will lead to an increased understanding of convective processes in the Earth System and to specific applications.

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Line C2. Optimization and parallelization of a new non-hydrostatic dynamical core for use in high resolution climate models

The next frontier in regional climate modeling is the development of models that can reach the convection permitting horizontal resolution of 1-5 km and can thus provide climate information at scales more relevant for impact applications. This requires the use of efficient and scalable non-hydrostatic dynamical cores in climate models so that long climate runs at these resolutions can be conducted. Towards this goal, a new non-hydrostatic dynamical core is being developed at ICTP, based on a finite element, semi-lagrangian, semi-implicit numerical framework, which is highly accurate without having stability constraints. A key aspect of this development is the capability of this code to scale efficiently on massively parallel machines. The aim of this project is to optimize the code of this dynamical core in order to make it highly scalable on different HPC platforms and thus applicable in a wide climate modeling context, including the new version of the ICTP regional model RegCM5.

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Line C3. Physical-Biogeochemical online coupling for Mediterranean Sea

One of the main HPC challenges in oceanography modelling is the increase of the model spatial resolution to potentially allow more realistic simulations of the coastal areas. In an exascale paradigm, a multi-model approach will be able to simultaneously simulate the Mediterranean Sea at different spatial resolutions and on different sub-regions, conveniently

calibrating the resolution increment and the boundary conditions between the basin and sub-basin scales. Online coupling between physical and biogeochemical components is envisaged as one of the issues to be tackled
The goal of this research line is to start developing an online coupling between biogeochemical and physical models for the Mediterranean Sea to be applied both for operational applications and climate projections. Background experience for the present activity is the online coupling between MITgcm and BFM implemented at OGS for the Northern Adriatic Sea with collaboration of UTMEA-CLIM section of ENEA.
The perspective view is the development of a regional system for operational forecasts specifically designed for the Northern Adriatic Sea, including numerical models (coupled model physics-biogeochemistry, eventually extended to upper trophic levels) and observational data sets necessary for data assimilation (of surface chlorophyll, in-situ data, surface currents).

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Line C4. Development of a library of HPC tools for the parallel implementation of p-adaptive discontinuous finite element methods applied to geophysical flows

Discontinuous finite element methods have been gaining in popularity for large scale geophysical applications. They are also a natural environment to take advantage of adaptive approaches in which the degree of the approximating polynomials is chosen locally and dynamically, in order to minimize memory occupation and computational cost. However, this poses major challenges to the parallel efficiency of the resulting methods, since a greater effort to achieve optimal load balancing is required. At present, no general HPC infrastructure for efficient and natively adaptive implementation of DG methods on massively parallel is available.
The purpose of this research line is to move towards the development of such a tool especially tailored for the simulation of fluid dynamics problems in climate dynamics, oceanography and volcanology. This development will rely heavily on the preliminary results already achieved in the previous cooperation among the proponents.

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Line C5. Numerical modeling of post-Last Glacial Maximum deglaciation of a marine-based paleo-ice cap

To look at processes leading to climate fluctuations in the past can significantly contribute to understand the present - and, possibly, to predict the future - climate variability under the dramatic conditions of climate change we are witness of.
For the reconstruction of the dynamics history of palaeo ice sheets-streams-shelf systems it is crucial the parametrizations in ice sheet models of climate forcing, surface mass balance and basal melting/refreezing under the ice shelves and other processes (for instance calving and basal hydrology) at the geometric boundaries of the ice sheets. The ice-ocean interaction and

investigation of the sensitivity of the ice shelf/stream retreat to ocean temperature are crucial to reconstruct the deglaciation scenario.
The aim of this research is to model the post-Last Glacial Maximum (LGM) deglaciation of a marine-based paleo-ice cap in the Arctic. In particular, we would like to focus on the Storfjorden and Bear Island ice streams, for which marine geological evidence suggests that they played an important role in the retreat of the Svalbard/Barents Sea Ice Sheet (SBIS) from the continental shelf edge during the last deglaciation. The relatively small (compared to other LGM glacial systems) catchment area of the ice cap should reflect in a more rapid response to climatic changes. We are interested in modelling the flow of the ice from the drainage area (Bear Island and Spitsbergen Banken) and we wish to investigate the Grounding-Zone Wedges formation and the meltwater production, possibly comparing the modelling with existing data. In order to model a glacial system (including ice streams and ice shelves, the so-called fast-flowing areas), to use a multiflow ice model is necessary.
For this research, it is needed to perform a large number of simulations (200-300) and an High Throughput problem occurs. Moreover the output of one simulation would be of the order of few GB; 200-300 simulations would produce huge outputs. One simulation (running on one processor with 20 km resolution) would take approximatively one week. For this reason HPC can greatly support this activity.

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Line C6. Development and optimization of a three-model chain (RegCM-CHyM-CA2D) to estimate the climate change impact on the flood hazard for the Euro-CORDEX region.

Regional climate modeling research is rapidly moving towards the development and application of fully coupled Regional Earth System Models (RESMs) including different components of the climate system, such as the atmosphere, oceans, land, sea ice, marine and atmospheric biogeochemistry. The Earth System Physics section (ESP) of the International Centre for Theoretical Physics (ICTP), develops and distributes to a large scientific community such a RESM system, based on the RegCM regional modeling framework. The ICTP RegCM-ESM model currently includes coupled atmosphere (RegCM4), ocean (MIT-GCM), land (CLM4.5), hydrology (CHyM) and chemistry/aerosol components. However the direct coupling between the river routing component and the hydraulic component is not yet available. Therefore the need is there to complete this coupling using physically based hydraulic model. The purpose of this line of research is thus to develop and optimize a three model chain that encompass the atmospheric regional climate model RegCM, the hydrological model CHyM and the hydraulic model CA2D.
Using as input meteorological variables produced by the RegCM4 (e.g. temperature, precipitation or surface and subsurface runoff), along with topographic information from a Digital Elevation Model, CHyM can calculate realistic discharge from river basins, which in turn generates an input (discharge) for the hydraulic model. This coupling requires extensive computing resources due to the complexities of all the individual components, and it thus critically relies on an efficient implementation on different HPC platforms.

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Line C7. Development of a High Performance hydrological model

The GEOtop hydrological scientific package is an open-source integrated hydrological model that simulates the heat and water budgets at and below the soil surface (http://geotopmodel.github.io/geotop/). It describes the three-dimensional water flow in the soil and the energy exchange with the atmosphere, considering the radiative and turbulent fluxes. Furthermore, it reproduces the highly non-linear interactions between the water and energy balance during soil freezing and thawing, and simulates the temporal evolution of snow cover, soil temperature and moisture. The core components of the package were presented in the 2.0 version (Endrizzi et al, 2014), which was released as Free Software Open-Source project. Recently, in the framework of the HPC-TRES MHPC master program, a code version 3.0 was released (Bortoli et al, in prep.). A software reengineering was performed: the code was translated in C++, and new efficient data structures were introduced to create a robust and stable scientific open software package. This research line aims (I) to improve code modularity to manage in a flexible way a complex state-of-the-art hydrological model like GEOtop and integrate it into wider workflows, as weather forecast or regional climate models; (II) to perform a code parallelization using a mixed OpenMP/MPI approach, with the implementation of numerical codes for parallel computation of the surface energy budget and of the Richards equation.

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Line C8. Development of a Regional Earth System model for the Northern Adriatic Sea area

A new challenge in climatology is a realistic representation of the complete Earth System, which takes in account all the climate components (atmosphere, ocean, land, cryosphere, biosphere, including humans) and the relationships among them.
Earth System models represent the state of the art in climate modelling: they have been initially developed for global approaches, and are now being used to reproduce the climate in regions characterized by particular sensitivity to climate change, such as the Mediterranean basin and its sub-regions. Reducing the investigated area, indeed, may constitute a compromise between the reduction of the model domain and the increase of the model complexity and resolution, thus decreasing the computational load required to simulate climate scenarios.
Following this approach, we recently parametrized and tested over the Northern Adriatic Sea area the regional Earth System model RegCM-ESM developed by the Earth System Physics section of the International Centre for Theoretical Physics (ICTP). The components of the climate system included in the Northern Adriatic Sea version of RegCM-ESM (RESM-NAd) are: atmosphere (RegCM4.7, 3 km resolution), oceans (MITgcm, 700 m resolution), rivers (CHyM, 3 km resolution), land (CLM4.5). The next step will be the inclusion of marine biogeochemistry module (BFM).

The initial purpose of this research line is to build up a realistic reference dataset at high resolution for the present physical and biogeochemical state of the North Adriatic Sea area. Then, RESM-NAd will be used to simulate high resolution future climate scenarios, comparing the projections with the present state.
As a by-product, the CHyM hydrological model implemented in RESM-NAd will be also exported to specific downstream services for the Northern Adriatic Sea (nested into the regional forecasting system for the Mediterranean Sea framed within the Copernicus Marine Environment Monitoring Service - CMEMS). This will potentially improve the quality of the biogeochemical products in the coastal areas, beneficial for the coastal monitoring services and for the interactions between regional and coastal systems.
Our high resolution simulation with RESM-NAd requires an intense computational effort: in the present configuration (288 cores on Galileo facility hosted at Cineca) one month of RESM-NAd simulation takes almost one day (i.e. 6912 core-hours; SYPD = 1/12), for five years it takes approximately two months. Though we are oriented to optimize the time-to-solution of RESM-NAd (using a new non-hydrostatic dynamical core of RegCM), the use of HPC remains fundamental.

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Topic D: HPC for Climate Sciences

Line D1. Climate studies of natural drivers and anthropic pressures on Mediterranean Sea marine ecosystems

Mediterranean Sea is an extremely heterogeneous sea basin in terms of physical forcings and biodiversity, and can be considered as a very sensitive area to the climate change effects on its ecosystems. The projections of the socio-economical effects related to climate change can be provided by integrated regional modelling (or Regional Earth System modelling), based on the coupling between ocean-atmosphere models, biogeochemistry models that involve the whole trophic chain, from plankton to big predators ("End2End" models), and socio-economical models. This approach, partially implemented in some EU-projects (e.g. PERSEUS, OPEC), is characterized by the computational challenge that could efficiently support simultaneously interacting, inter-dependent codes running on high-resolution grids for multi-annual integration periods, and that produce large amount of data.
Given the high uncertainty related to the sensitivity of the biogeochemical models to their parameters, the aim of this research line is the exploration of an ensemble of multi-decadal simulations (generated according to different initial and boundary conditions) of the Mediterranean Sea biogeochemistry, in order to evaluate the impact of the natural drivers (linked to climate change) and anthropic pressures (linked to environmental policies) on the marine ecosystems. This topic is extremely strategic in the frame of the Marine Strategy Framework Directive (MSFD)[5].

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Line D2. High-resolution ensemble global climate simulations

The reconstruction of past climatic fluctuations is an essential step to obtain the baseline of climate variability against which to project current climate change. Several proxy records are now available for the last few Millennia, with a specific focus on the past 2000 yr, as for example indicated by the international PAGES-2k initiative. Parallel to the proxy data reconstructions, simulations of climate variability in the last Millennia are necessary. Technically, however, such simulations - if performed at high spatial resolution- require HPC approaches, since one single simulation is not sufficient and an ensemble of possible climatic histories is usually needed. This research project focuses on the implementation, tuning and use of the high-resolution global climate model EC-Earth for ensemble paleoclimate simulations. The goal is to obtain an ensemble of high-resolution (0.75°) simulations of global climate in the last 2000 years with different solar and land-use forcing reconstructions, to obtain estimates of natural climate variability in the centuries before anthropogenic greenhouse gas emissions.

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[5] http://ec.europa.eu/environment/water/marine/directive_en.htm

Line D3. Coupling of marine biogeochemical models to a regional Earth System model framework

The interest is steadily growing within the regional climate modelling community on the development of fully coupled Regional Earth System Models (RESMs), aimed at addressing climate system interactions at the regional to local scale. Within this context, a component noticeably missing in most current RESM efforts is marine biogeochemistry, which on the other hand is of high interest in global change studies.
In particular, ICTP is currently developing a coupled RESM including atmosphere (RegCM), ocean (MIT-GCM) and land (CLM) components. At the same time, OGS has developed and used a range of marine biogeochemistry and ecosystem models, so that a clear opportunity exists to develop a collaboration aimed at the integration of a marine biogeochemistry component within the ICTP regional model system.
Target of this project is to carry out such an exercise with specific applications to the Mediterranean region, addressing in particular the issue of the sensitivity of coupled processes to the complexity of the biogeochemistry model components.

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Line D4. Role and effects of air-sea coupling in the climate variability of the Mediterranean Sea

Ocean mesoscale in the Mediterranean Sea is characterized by a Rossby deformation radius of 5-10 km. In consequence, the SST often shows narrow and sharp fronts as well as filaments with associated strong temperature gradients that can significantly modify the air-sea interaction and affect the climate evolution. Ocean mesoscale also plays a crucial role in the main mechanism of heat uptake by the ocean, namely dense water formation, which modelling requires both atmospheric and oceanic high spatial resolution that present GCMs are not able to achieve. A detailed analysis of how air-sea coupling at high resolution can modify the regional climate, and consequently the global climate, is still missing in the literature. There are some indications that it can provide an added value to RCMs in both present climate and future scenarios, but the mechanisms underlying such impact are not completely understood. Global climate modelling should therefore benefit from this research line as it will give clues for the future design of GCMs. This research line aims to highlight the role played by air-sea coupling in both regional climate variability and future projections for the Mediterranean area.
This research project focuses on the tuning and use of a state-of-art Euro-Mediterranean regional climate model for hindcast and future climate simulations in the context of the recently approved CORDEX Flagship Pilot Studies. The regional climate model is composed by RegCM4 and MITgcm interactively coupled via ECMF tool. The goal is to perform a set of climate simulations for evaluating the impact of high-resolution ocean component on air-sea coupling. Both present and future climate simulations will be performed with the ocean component at a resolution of 1/16º with a 1/64º zooming in the main straits (i.e. Gibraltar).

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Line D5. High resolution simulations of extreme meteorological events

Heavy rains, hurricanes, wind storms constitute major hazards for populations and societies. Our ability to predict them is severely limited and modelling frameworks are an important tool for understanding the relative role of individual processes and mechanisms involved in their development. Different aspects will be investigated in this research line, including the role of orography in enhancing precipitations, the direct and indirect effects of aerosols on cloud formation and stability, the two-way interaction with the sea surface and its role in affecting air stability and wind intensity as well as upper ocean mixing and internal wave propagation. The investigations will be performed by means of atmospheric models, regional ocean models, and coupled models, both in idealized and realistic configurations. The present line presently includes 2 tasks.
Task 1 "Air-sea interactions at the submesoscale" - The upper ocean responds passively to the atmosphere at large scales, where winds are negatively correlated with sea surface temperatures. At smaller scales, the atmosphere responds to sea surface thermal structure and currents by modifying the near surface wind and the boundary layer stability depending on enthalpy and momentum air-sea fluxes. In turn, the submesoscale structure generates intense vertical motion that impact the redistribution of heat and nutrients in the upper ocean. In this project, small scale interactions between the atmosphere and the ocean will be investigated using the regional ocean model ROMS and the atmospheric model WRF either in standalone or in coupled configurations, in some cases including a wave model at the interface. Part of the project is done as a study for the ESA Earth Explorer 9 prospective mission"Harmony" (formerly known as Stereoid).
Task 2 "Extreme meteorological events in the Alpine region". - The scientific activity consists in performing high resolution numerical simulations of selected heavy rain events in the Great Alpine Region. This will allow the study and the understanding of the convective scale processes that often contribute to the intensification of the precipitations, even in cases triggered by frontal dynamics and/or orographic lifting. Outputs from the state-of-the-art global climate model EC Earth performed following the CMIP5 protocol, available at 25, 40 and 80 km resolution for 30-year long intervals both for the historical period (1979-2008) and for the RCP8.5 scenario (2041-2070), will be used as boundary conditions for a dynamical downscaling experiment using the Weather and Research Forecast model on a 4km x 4km grid over the Great Alpine Region. The model will be run for the 30 year long periods described above for different simulations of the present and future climate ensembles. Up to three two-way nested domains will be used, to downscale from the grid spacing of EC Earth to the 4 km grid spacing, using intermediate domains such that each domain reduces the grid size of about a factor 3 from the coarser one.

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Line D6. Ensemble simulations of paleoclimates, extreme climates and exoclimates

Climate dynamics on Earth has been characterized by large variability, going from Snowball conditions, when the planet was largely covered with ice, to the equable climates of the Cretaceous and Paleogene, that was several degrees warmer than the current conditions with a small temperature difference between the poles and the equatorial regions. Such past climates are formidable test grounds for our understanding of the climate system, and need to

be described by comprehensive approaches including geological, biospheric, cryospheric, oceanic and atmospheric components. These extreme climates, as well as abrupt climate changes and shifts, can be studied by a hierarchy of models that range from simple, one-dimensional Energy Balance Models, to Earth System Model of Intermediate Complexity, to full-blown Global Earth System Models. Similarly, the climate on extraterrestrial planets and moons is a challenging scientific problem that requires the development of new ideas and parameterizations, describing the dynamics of atmospheres with a completely different chemical composition (Venus, Titan), flows in electrically-conducting ice-covered oceans (Enceladus, Ganymede, Europa), as well as issues related to planetary habitability and exoplanetary climates (for example, Kepler 452b).
The exploration of these challenging systems requires developing large-ensemble simulations taking into account all possible values of unknown parameters and forcing factors, thus fully residing in the area of High Performance Computing blended with the development of new approaches to the analysis of climate variability and dynamics.

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Line D7. Extreme rains in complex orography areas: high resolution meteorological modelling on heterogeneous computing architectures (high performance computing, cloud computing, grid computing)

The extreme precipitation events in complex topography regions, such as coastal areas of the Mediterranean sea, can produce, especially in densely urbanized areas, sudden floods with high socio-economic impacts. The climate change effects already under way will contribute to exacerbate this situation, making such events likely more frequent.
The specific objective of the research activity is therefore the development of a system that supports the characterization of extreme precipitation events in areas with complex topography, with the ultimate aim of contributing to improve the hydro-meteorological early-warning systems.
The system must be able to use both data acquired in real time and historical datasets for the reliable and timely execution of high-resolution meteorological simulations (about 1 km), also supported by data assimilation techniques and in probabilistic multi-physics mode, on high-level computing systems performance and cloud computing infrastructure. In addition, the system must allow integration with various analysis and post-processing and data transfer procedures as well as further coupling with hydrological and impact modeling.

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Topic E: "BigData" in Earth Sciences

Line E1. Large scale data analysis for climate data

In several eScience domains the analysis and mining of large volumes of data is increasingly becoming central to scientific discovery. In particular, the multidimensionality, volume, complexity, and variety of scientific data require specific solutions able to (1) support the management and analysis of large datasets, (2) provide array-based functionalities, and (3) support the scientific analysis process through parallel solutions able to deliver results in (near) real-time.
The main objective of this research project is to identify, extend and apply scalable big data analysis solutions running data intensive tasks on High Performance Computing (HPC) machines to address scientific analysis needs and issues in (near) real-time. The work will relate to (1) requirements gathering concerning the analysis of large volumes of scientific data (e.g. climate/weather), with a specific focus on multidimensional datasets; (2) the analysis and identification of big data platforms suitable for scientific data analysis and visualization to perform a cross-domain evaluation; (3) the extension and customization of the selected big data platforms for climate datasets, to support a large number of scientific use cases; specifically, these platforms will address scalability in terms of new storage models and data partitioning, efficiency in terms of parallel solutions and interoperability requirements by adopting well-known standards at different levels (data formats, communication protocols, etc.).

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Line E2. Map-reduce approach to Regional Climate modelling pre/post-processing activities

This proposal refers to the idea of evaluating some of Big Data tools/techniques developed for big data activities for industry, in the scientific area of Earth Science. More specifically the goal of this proposal is to test and investigate the use of Hadoop, a widely used Big Data framework, its Distributed File System (HDFS) and its MapReduce data-driven computational engine to run the preprocessing and the post-processing phase of a climate experiment involving a regional climate modeling tool on a HPC cluster.
In the context of Climate modeling, a considerable amount of time is spent in processing huge volume of data, either in preparing model input and analyzing the large amount of data produced by the simulations. Application codes used to process the data are usually written in Fortran language, and most of the datasets used in the climate modeling community are in the NetCDF format making the adoption of Hadoop not straightforward at all [1].
To achieve the overall goal Hadoop's logic should be modified to allow in a transparent way both 1) code execution using all the pre/post processing tools and 2) dataset management on HDFS without any modification on the original dataset. To standardize the execution environment on Hadoop, and to make the approach as much portable as possible, the usage of Container-based Virtualization with Docker will also be considered.
The proposed case study will focus on the RegCM Regional Climate Model tool developed by the ICTP and its preprocessing and post-processing programs, but the success of this project would bring benefits also to the entire Earth Science community when dealing with similar use cases, and to the wider extent of filling the gap between modern Big Data platforms and scientific codes in general.

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Line E3. Data management, preservation and curation activities of the National Oceanographic Data Center (NODC)

EMODNet Chemistry (coordinated by OGS) is the European Marine Observation and Data network focused on the groups of chemicals relevant for MSFD Descriptors 5, 8 and 9, aiming to unlock and make available European marine data resources from diverse sources in a uniform way.
The assembled data, data products and metadata are hosted on a structured repository on a cloud environment, made available by CINECA. A series of nodes presently host horizontal gridded maps produced with DIVA (Data-Inverse Variational Analysis) made available through an in-house WMS service and in-situ data, properly discovered, analyzed and visualized with a standard, OGC compliant, WPS service. The data discovery and access service enable users to have a detailed insight of the availability and geographical extent of archived data. This repository hosted in the CINECA cloud represents a wealth of information scientifically aggregated and validated, accessible via the EMODnet Chemistry portal.
The Italian National Oceanographic Data Center (NODC) managed by OGS is going to be replicated at CINECA, together with a web service environment to satisfy the needs of European projects asking for continuous access to data and metadata and national collaborations.

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Line E4. Optimization of vegetation sun-induced fluorescence retrieval from hyperspectral airborne/satellite remote sensing

Spectral fitting method (SFM) is an accurate method to retrieve vegetation sun-induced fluorescence (SIF). The SIF represents a novel remote sensing tool for monitoring plant status (and plant productivity) that can improve our understanding of canopy-atmosphere energy/matter. The SFM is currently under implementation/development for the forthcoming ESA's 8th Earth Explorer mission FLEX (Fluorescence Explorer, scheduled launch 2021) to provide SIF observations and geophysical products at global scale. The SIF retrieval by SFM relies on the inverse decoupling (non linear least squares) of surface reflected radiance and sun-induced fluorescence from spectrally resolved radiance spectra. The exploitation of SFM on a large dataset of high-resolution imagery collected either by airborne HyPlant airborne hyperspectral sensor (i.e. the airborne demonstrator of FLEX) or satellite spectrometers will benefit by high performance computer approach.
The main aim of the project consists in implementing an operational SIF retrieval processor for airborne and satellite imagery. The scientific activity consists therefore on: i) reviewing currently available technical parallel software and infrastructures; ii) implementing SFM in efficient computer language (i.e. C, C++, FORTRAN); iii) selecting and implementing SIF retrieval at image scale by using parallel computation approach on hyperspectral airborne and satellite data (e.g. Tropomi).

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Line E5. Analysis and modelling of large-scale datasets from seismology and geophysics

The intention is to improve our capacity of processing and analyzing large volumes of data or reanalyzing data repeatedly in an efficient way in order to allow for the full exploration of the parameter space. Therefore, we are developing innovative platforms for large scale data analysis (Big Data) and are combining these with well-established processing and analysis algorithms used in seismological and geophysical research. We anticipate that the availability of efficient and scalable tools will lead to the development of innovative analysis methods, which were not accessible before.
This research project proposes to develop and implement a Data Analytics platform, and to apply, adapt and evaluate tools from the Big Data / Data Analytics environment for the processing and analysis of big volumes of seismological and geophysical data. We intend to use products from the Apache Hadoop ecosystem, especially Apache HDFS, Spark, Flink, HBase, MongoDB to create new scientific or operational applications or to port existing applications onto this platform.

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Line E6. Application of the wave equation datuming for marine seismic data

The quality of reflection seismic data is very important for seismic processing and interpretation. It depends on factors, such as the seismic characteristic of the Earth's surface, complexity of the subsurface, and technical equipment used in the acquisition stage. The quality of vintage seismic reflection data, which needs to be reprocessed, often is comparably low because of the short maximum offsets, and low common-midpoint (CMP) fold. It is clear that it is necessary to apply advanced techniques to obtain more information. So, our target is to apply our experience on Wave Equation Datuming (WED) in order to extract more information from available seismic data. It is important to note that the data will be processed following a non conventional procedure to preserve the relative amplitudes of the reflections and to better investigate the subsoil structures.
WED can contribute to increase the signal/noise ratio reducing the coherent and incoherent noise. So, it is necessary to perform a systematic and deep study in other dataset in order to optimize the procedure and increase the seismic imaging. This research line proposes to apply the WED in different offshore seismic dataset acquired. In particular, we propose to study the WED in the following cases: 1) shallow water where the multiple and refraction events are a strong noise and masks the primary reflections (the target of seismic acquisition); 2) areas with complex geometries that can cause strong lateral events masking the primary reflections; 3) areas characterized by strong diffractions, generally difficult to attenuate by using standard processing, which mask deeper reflections.
The WED is applied by using the open-source software Seismic Unix (SU) and the seismic dataset is vintage seismic data available at OGS. The aim is to relocate the shots and the receivers to a new datum applying WED equation. Basically, WED is the process of upward or downward continuation of the wavefield between two arbitrarily-shaped surfaces. The

characterization of the velocities is crucial for WED computations and a proper procedure is to define the seismic velocity field by tomographic inversion or by using pre-stack depth migration iteratively. In our case, the input seismic data are processed accurately in order to attenuate the noise and increase the signal/noise ratio. Applying the WED to the processed seismic data by using the seismic velocity, we obtain an improved stacked section, which can help in the interpretation of the seismic data. In fact, the so-obtained seismic section will be a higher vertical and lateral resolution with respect to the conventional stacked section.
Recently, we started to use WED to improve the analysis and the interpretation of the seismic data acquired in presence of gas hydrate and free gas reservoirs. This topic is very timely because the stability and the presence of the gas hydrate could have a strong impact on climate change, geohazard and energy resource. The seismic imaging of the gas hydrate and free gas presences after the application of this approach allowed a better resolution of the complex geological features, such as the fluid flow. Moreover, the base of the free gas layer, generally masked due to peg-legs and strong attenuation, can be recognized more easily after the application of the WED.
The WED is rarely used in geophysical analysis for two main reasons: not all commercial software include this tool and powerful computational resources are required, due the complexity of the numeral computation. In fact, the WED resolves the wave equation sample by sample of all traces, combining the result in order to re-locate the energy at the right position. The present research line proposes to adopt an HPC approach to reduce the computational time-to-solution for the WED and therefore greatly increases the amount of data to be analyzed.

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Appendix

A1. Links to institutional web sites

1. CINECA: http://www.cineca.it/
2. OGS: http://www.inogs.it/
3. ICTP-Earth System Physics: https://www.ictp.it/research/esp.aspx
4. CMCC: http://www.cmcc.it/
5. INGV-Pisa: http://www.pi.ingv.it/
6. CNR/ISAC: http://www.isac.cnr.it/
7. CNR/IGG: http://www.igg.cnr.it/
8. MOX – Politecnico di Milano: https://mox.polimi.it/
9. ENEA – Dip. Sostenibilità dei Sistemi Produttivi e Industriali: http://www.enea.it/
10. INGV – Centro Nazionale Terremoti: http://cnt.rm.ingv.it/
11. INGV – Sezione Sismologia e Tettonofisica: http://www.roma1.ingv.it/
12. Univ. Bicocca – Dip. Scienze Ambiente e Territorio: http://www.disat.unimib.it/
13. CRS4: http://www.crs4.it/research/energy-and-environment/imaging-and-numerical-geophysics/
14. EURAC: http://www.eurac.edu/
15. ARPA-FVG: http://www.arpa.fvg.it/
16. CIMA: https://www.cimafoundation.org/
17. Univ. Trieste – Dip. Matematica e Geoscienze: https://dmg.units.it/
18. Univ. Trieste – Dip. Ingegneria e Architettura: https://dia.units.it/