2nd Workshop HPC-TRES

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Training and
Research for
Earth
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2nd Workshop HPC-TRES

High Performance Computing – Training and Research for Earth Sciences
November 19th 2019, RTM Living ex-Ospedale Militare – Trieste, Italy

The HPC-TRES program

HPC-TRES is a national initiative promoted by OGS and CINECA aimed to implement a training program focussed on High Performance Computing (HPC) applications for Earth Sciences. HPC-TRES 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.

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, lithosphere 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, the HPC-TRES program establishes, sponsors and oversees training and research awards (in the form of scholarships grants) that support the research lines described in the scientific plan of the HPC-TRES program. A number of Italian research groups and institutions involved in HPC applications for Earth Sciences (INGV-Pisa, CNR/ISAC, CNR/IGG, CMCC, ICTP-ESP, MOX-Politecnico di Milano, ENEA-SSPT, INGV-SST, INGV-CNT, Univ. Bicocca, CRS4, EURAC, ARPA-FVG, Fondazione CIMA, Univ. Genova, Univ. Trieste) have already endorsed the HPC-TRES initiative, contributing to the HPC-TRES scientific plan.

The 2nd HPC-TRES workshop

The 2nd workshop of HPC-TRES was organized by OGS at the “RTM Living ex-Ospedale Miltare”, Trieste. The main objectives were: to gather all the research groups that contributed to the HPC-TRES scientific plan, to present the status and the current outcomes of the research activities, to highlight the future perspective of the national HPC infrastructure and to offer an opportunity of discussion and cross-discipline contamination, supported by the common HPC background which characterizes the different scientific approaches adopted by the research groups involved in the program.

A total of 33 participants registered to the workshop, and 18 past and present HPC-TRES grantees (53% of the total grants acknowledged by the program in the period 2014-2019) presented the main results of their research work, highlighting the scientific and technological challenges they have coped with. Modelling studies at different spatial and temporal scales, implementation of innovative algorithms, model optimization, HPC model data management, covered different Earth Sciences topics: from global to regional climate, atmosphere, ocean, hydrology, volcanic and earthquakes studies.

Tab. 1 shows the list of participants, some information related to the reference HPC-TRES research line where they are involved, and the title of the presentations. The abstracts of the presentations are included in the present report.

	Name, institution	Notes (role, research line, title of presentation)
1	Cosimo Solidoro, OGS	Steering Committee, President (A1, A2, A3, A4, C3, D1, D3)
2	Filippo Giorgi, ICTP	Steering Committee (C2, C6, D3)
3	Jost von Hardenberg, ISC-CNR	Steering Committee (D2)
4	Tomaso Esposti Ongaro, INGV	Steering Committee (B5, B6, B7, C4)
5	Stefano Salon, OGS	Steering Committee, Secretary (A1, A2, D1)
6	Julie Baron, OGS	Simulazioni degli effetti topografici in Arquata del Tronto (B1)
7	Giacomo Bertoldi, EURAC	Towards a HPC version of the GEOtop hydrological model code (C7)
8	Federico Brogi, INGV	MagmaFoam, a Versatile Computational Tool to Simulate Magmatic Processes (B6)
9	Stefano Campanella, OGS/EURAC	Development of a High Performance Hydrological Model (C7)
10	Philippe Cance, OGS	Modeling of seismic and electromagnetic waves (B14)
11	Mattia Carello, OGS/UNIBO/CRS4	Imaging and numerical geophysics (B10)
12	Florence Colleoni, OGS	Paleo-modelling of the Antarctic ice sheet: preliminary results and challenges (C5)
13	Nicola Creati, OGS	(B4)
14	Alessandro D'Anca, CMCC	(E1)
15	Eleonora Denich, UNITS/OGS	Numerical methods for Full Waveform Inversion. Analysis and implementation (B3)
16	Marco De Pasquale, ESTECO	My journey from Academia to Industry (A2)
17	Valeria Di Biagio, OGS	MITgcm(BFM) focus on marine biogeochemistry: emerging scales of variability (C3, D1)
18	Fabio Di Sante, OGS/ICTP	Il modello climatico regionale accoppiato atmosferico-oceanico-idrologico RegCM-ES: stato attuale e sviluppi futuri (C6)
19	Davide Gei, OGS	(B14)
20	Mostafa Hamouda, Univ. Bicocca	A breakdown of the link between AO and NAO in warmer climate projections (D5)
21	Peter Klin, OGS	(B1, B2)
22	Arnau Mirò, OGS	3D visualization of the Mediterranean Sea (A1)
23	Chiara Montagna, INGV	(B6)
24	Paolo Novati, UNITS	(B3)
25	Stefano Parolai, OGS	(A7, B12, B13)
26	Eric Pascolo, CINECA	Utente vs Exascale computing: la prospettiva CINECA per HPC-TRES (A1, A4)
27	Claudia Pasquero, Univ. Bicocca	(D5)
28	Giovanni Petris, UNITS/OGS	Hydroacoustic models for environmental applications (A7)
29	Marco Reale, OGS	(Extreme) synoptic patterns and biogeochemical dynamics in the Mediterranean Sea (D3)
30	Chiara Scaini, OGS	Calculation of damage maps for seismic scenarios in Friuli-Venezia Giulia, Italy (B12)
31	Aldo Vesnaver, OGS	(B3)
32	Luigi Sante Zampa, UNITS/OGS	Gravity data reduction and inverse modelling in compressional and extensional geodynamic settings (B11)
33	Maria Zanenghi, OGS	Logistic Support

Tab. 1 – List of participants (with affiliations), and notes including role, HPC-TRES research lines, and title of presentation. Enrico Pochini and John Ford, PhD students at UNITS/OGS were present as auditors.

Acknowledgement

The 2nd HPC-TRES workshop was supported by OGS thanks to the MIUR grant "PRACE-Italy", under the extraordinary contribute for the Italian participation to activities related to the international infrastructure PRACE – The Partnership for Advanced Computing in Europe.
We acknowledge Maria Zanenghi (OGS) for the logistic support for the workshop organization.

The HPC-TRES Steering Committee:
Cosimo Solidoro (OGS, Trieste)
Filippo Giorgi (ICTP, Trieste)
Tomaso Esposti Ongaro (INGV, Pisa)
Antonello Provenzale (CNR-IGG, Pisa)
Giovanni Aloisio (Univ. Salento and CMCC, Lecce)
Jost von Hardenberg (ISAC-CNR, Torino)
Carlo Cavazzoni (CINECA, Bologna)
Stefano Salon (OGS, Trieste)

References

HPC-TRES program, web page:
http://www.ogs.trieste.it/en/content/hpc-training-and-research-earth-sciences-hpc-tres

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47	Zampa, L.	Gravity data reduction and inverse modelling in compressional and extensional geodynamic settings

3D numerical modeling of topographic seismic site effects: application to Arquata del Tronto, Italy

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Keywords: seismic ground motion, numerical simulations, spectral element method, topography

In this study, we use 3D numerical modeling of seismic waves propagation in order to put in evidence possible effects of topography on the earthquake ground motion in the specific case of Arquata del Tronto, a municipality located in the epicentral area of the 2016 seismic sequence, that hit the Central Apennines with four Mw>5.7 mainshocks. During the sequence, Arquata del Tronto was characterized by a clear spatial variability in the maximum observed seismic intensity, which ranged from VII MCS (very strong) in the Borgo settlement to IX MCS (destructive) on the Arquata del Tronto ridge. Similar variability was observed also in other settlements in the area, which are located on the top of a hill or a ridge, thus raising the question of the possible role of topography in earthquake ground motion amplification in these cases.

Site effects are defined as modifications, in terms of frequency content, amplitude and duration, that an incoming seismic signal is subjected to, as the seismic wave interacts with the topographic surface and local subsurface structure. In order to evaluate the interactions of the seismic wavefield with an irregular topographic surface and subsurface structure we have to rely on numerical solutions of the elastodynamic wave equation in 3D.

We analyzed the site effects in Arquata del Tronto in terms of 3D transfer functions, i.e. the seismic ground motion, that corresponds to three vertically incident plane waves polarized along each of the three spatial directions (Est-West, North-South, Up-Down), as suggested in Paolucci et al. (1999). The analysis was done both on a reference homogeneous (Vs=1000m/s) model of the subsurface and a 3D heterogeneous model, that was set up in collaboration with a research group from the University of Chieti, using the geological and geophysical information that was available for the Arquata del Tronto site. The 3D model is characterized by the alternation of Vs=900m/s and Vs=1000m/s layers and includes a thin superficial weathering layer of Vs=700m/s and a small basin with Vs=450m/s in the valley underlying the Borgo settlement.

Numerical simulations of seismic waves were performed using the open-source software SPECFEM3D (Komatitsch et al. 2002a; Peter et al. 2011), which is based on the spectral element method. The code accounts for intrinsic attenuation properties of the medium and avoids reflection effects from the spatial domain boundaries thanks to the usage of Perfectly Matched Layers. In our case the spatial domain consists in a 3D mesh of 518.400 hexahedral spectral elements, with size ranging from 25m at the topographic surface, which reaches 800 m a.s.l., to 50m at the flat bottom surface, set at -500 m a.s.l. The spatial domain covers a square area of 3x3km$_2$ oriented in the east and north direction respectively and centered on Arquata del Tronto hill. To generate the incoming planar seismic wave, we place a carpet of point sources at -400 m a.s.l. The ground motion is recorded in a dense network (20 m spacing) of virtual seismic stations over a 1km2 square area centered on the Arquata del Tronto hill. Considering the velocities of the seismic waves, the discretized spatial domain allows us to compute ground motion in the frequency band [1-10] Hz, which is typically associated with the damage potential of the ground shaking for common buildings.

Simulations were done using the computing resources at CINECA, that were available from an IscraC project. The computational jobs consisted in 225 MPI tasks, distributed on 5 knl nodes with 45 tasks-per-node on the Marconi super-computer. The simulations required a preprocessing step (mesher), which consists in building the computational mesh and assigning its geophysical properties and boundary conditions and which required around 225 CPU hours. The proper job regarding the resolution of the wave equation on each point of the computational grid (solver) required around 900 CPU hours to produce 8 seconds' long seismograms sampled with a time step of dt=0.0005 s.

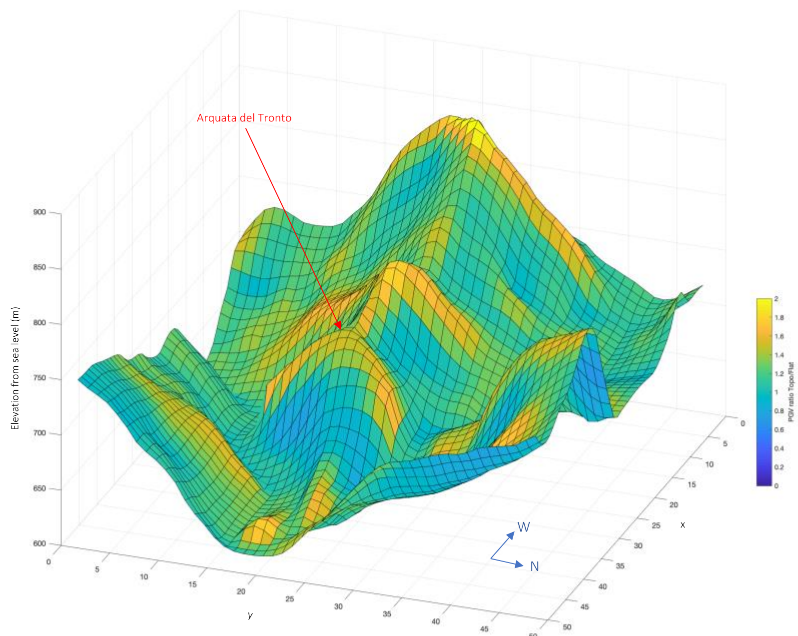

Figure: Peak Ground Velocity (PGV) ratio distribution over the study area of Arquata del Tronto. The distribution refers for an E-W polarized seismic input in the 3D geophysical model. Maximum amplification is observed on the crest oriented in the North-South direction (direction perpendicular to the polarization of the incoming seismic waves).

In the simulated waveforms, we observed a clear effect of the topography on the amplitude and duration. As we can see in the Figure, the distribution of the Peak Ground Velocity (PGV) ratio, computed as the PGV from topography with respect to the PGV from the reference flat model, clearly shows a variability of the ground motion amplification with respect to the topography surface. In particular, the horizontal components of the seismic ground motion signal evidence the highest amplification on the crest oriented in a direction perpendicular to the polarization of the incoming seismic waves. Vice versa, considered an incoming wave polarized along the North-South direction, the amplification results maximum on the crest oriented in an East-West direction. Comparing the PGV ratio obtained with the homogeneous and 3D heterogeneous model, we also highlighted the enhancement of the observed topographic effects due to heterogeneous undersoil structure.

Acknowledgement

The research reported in this work is supported by OGS and CINECA under HPC-TRES program award number 2017-22. We acknowledge the CINECA award under the ISCRA initiative, for the availability of high performance computing resources and support (IscraC “SERATA”).

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Towards a HPC version of the GEOtop hydrological model code

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Keywords: GEOtop, hydrology, software engineering, integrated models

GEOtop (Rigon et al., 2006; Endrizzi et al. 2014) is an integrated hydrological model that simulates the heat and water budgets at and below the soil surface (Fig. 1). Typical examples of its applications include flood and drought forecasting, water resource management, agricultural productivity forecasting and climate assessment studies. The latest version of GEOtop (v 3.0) has been rewritten in C++ from C and its source code is available on GitHub with a GPL3 licence.

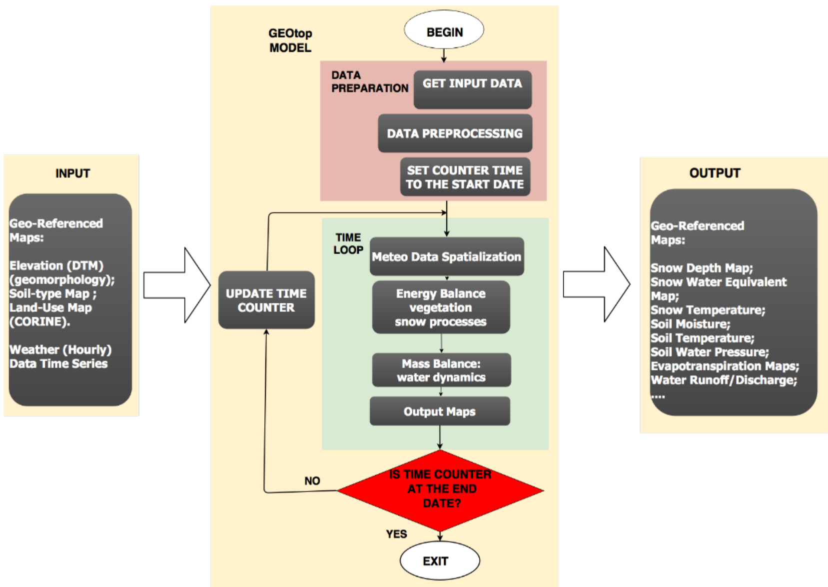

Fig.1 – Workflow of the GEOtop model code (courtesy of E. Cordano).

The development of this software spans over a decade and is the result of the layering of contributions from developers with different backgrounds and more emphasis on the scientific results than the code quality. Therefore, although being scientifically advanced, the codebase and documentation of this model suffer a big technological debt (something not uncommon among scientific software projects of this size) and the application has issues of performance and stability. In fact, software engineering techniques are often poorly implemented in hydrological models. This is a quite common issue in the scientific software community, which is facing a crisis created by the confluence of disruptive changes in computing architectures and new opportunities for greatly improved data availability a simulation capabilities.

Therefore, the GEOtop code has been re-engineered it the framework of a recent MHPC thesis under HPC-TRES program (Bortoli, 2018).

In particular, (I) a series of test cases for benchmarking have been made available for the developers community and included in a continuous integration mechanism (Travis-CI). (II) A code optimization has been performed introducing modern and more efficient data structures (from C to C++) and an optimization of the mathematical operations. (III) A testing suite for debugging and performance analysis (likwid-perfctr, unit tests, profiles) has been introduced.

In synthesis, the ongoing development of GEOtop is aimed at improving of both a high-productivity and high-performance hydrological model. In particular, in the framework the European Regional Development Fund (ERDF) project DPS4ESLAB, a near-real time model application for the estimation of the water budget has been realized. A preliminary implementation is available here: https://maps.civis.bz.it/ (Fig. 2).

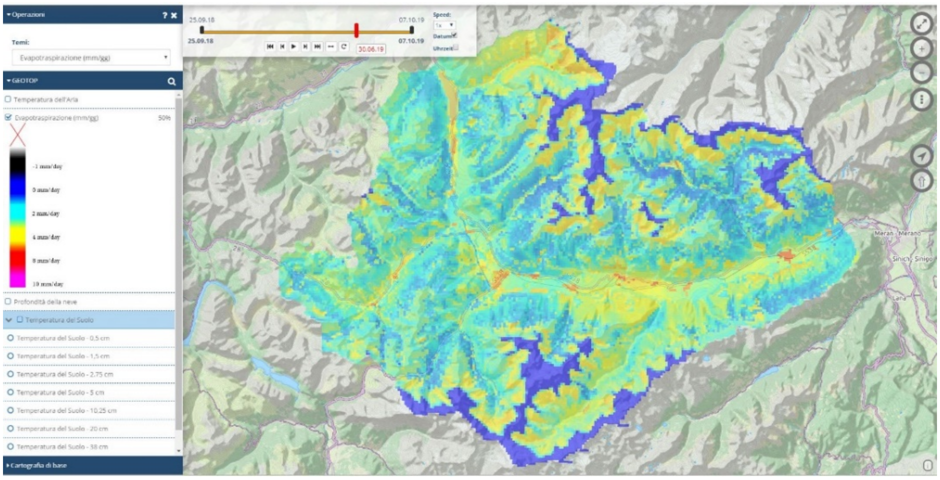

Fig.2 – Example of GEOtop model output from the online platform https://maps.civis.bz.it/. Map of actual evapotranspiration (mm/day) in the Venosta valley on the 30 June 2019

A new phase of development will be conducted approximately in the period spring-fall of 2020 within a MHPC thesis project (SISSA & ICTP), under the supervision of the cofinancing HPC-TRES sponsor Eurac Research. The planned goals are the following:

- Code reengineering
    - Code modularization with a better separation of I/O and data management from computation parts.
    - Implementing in the version 3.0 the MeteoIO libraries for better input data processing and spatialization (Bavay and Egger, 2014).
    - Replace custom linear algebra routines with standard BLAS/LAPACK packages
- Improve computational efficiency
    - Code parallelization with OpenMP to enable multithreading (e.g. in linear algebra and by parallelizing the energy/mass balance routines),
    - Code parallelization with domain decomposition (e.g for the energy balance, divide the domain in multiple 1D columns, for the water balance subdivide the catchment in subcatchments).
- Improve users productivity
    - More efficient I/O data storage using NetCDF or Data Cube to be easily manged with raster data management systems (http://www.rasdaman.org/)

- Capability to have in input downscaled climatic grids coming from meteorological or climatic models (Fiddes et al. 2019).
- Standardize the pre- and post-processing within a Python/Julia library, which, for example, could encapsulate and manage the GEOtop app;
- Create a framework/library in Python/Julia for launching multiple instances of GEOtop and make ensemble analysis (e.g. for parameter space exploration, coupling with stochastic meteorological models or training neural nets).

- Integrating external post processing tools with the version 3.0, preparing a set of working examples.
    - Developing of R and Python interfaces for I/0 management as geotopbircks (Cordano et al., 2015).
    - Optimization and sensitivity tools, as the R package gtopOptim (https://github.com/ecor/geotopOptim) or the GEOtop PEST interface (Soltani et al., 2019).

The ultimate goal of this project is of increasing usability, to ease further development and the integration with other packages and to enhance performances.

Acknowledgement

The research reported in this work was supported by OGS and CINECA under HPC-TRES program award numbers 2017-20 and 2019-33, by Eurac Research and by the European Regional Development Fund (ERDF) 2019-2021 under the project DPS4ESLAB.

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MagmaFOAM, a versatile computational tool to simulate magmatic processes

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Keywords: magma, modelling, multiphase

A better understanding of magma transport phenomena is of crucial importance not only to determine the eruptive potential but also to correctly interpret geophysical signals recorded by volcano monitoring systems that serve for forecasting the volcanic activity and volcanic hazard assessment. 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 silicate melt, solid crystal phases and exsolved volatiles, which ultimately determine the eruptive potential.

The progress in computer performances and improvements in numerical modeling techniques allow us to simulate more and more complex processes, describing multiphase-multicomponent systems in mechanical and thermodynamical disequilibrium. However, the growing complexity of the simulations requires more sophisticated approaches that can include specific constitutive models as well as dedicated solution techniques for the different dynamical regimes. The open source library OpenFOAM (OF) is the ideal platform on which we can develop our dedicated computational toolbox. In fact the OF modular object-oriented implementation (C++) allows the developers to easily expand and adapt the code and the users to combine different implemented models at run-time with almost no need to code. We developed the MagmaFOAM (MF) library on top of OF as a powerful dedicated toolbox to solve multiphase flows characterizing magmatic systems in general. The model can include thermo-mechanical non-equilibrium phase coupling and phase change between silicate melt and volatiles, state of the art multiple component solubility models and constitutive equations with real thermodynamic and transport properties. It retains the modular structure of OpenFOAM, and allows the user to select at run time different solution techniques depending on the physics of the specific process, thus optimizing available resources.

Current MF testing and applications focus on both pre- and syn-eruptive phenomena that are relevant to eruptions forcasting and monitoring. In particular, these include: buoyancy driven magma mixing (Figure 1a), magma-gas dynamics with phase change (e.g. exsolution of volatiles, Figure 1b), rapid decompression of gas-melt conduits (Figure 1c), ascent of large gas bubbles in open conduits (Figure 1d). A more detailed description of each simulation is given in the figure caption. These applications show the ability and versatility of MF in using dedicated modeling approaches to deal with different domains of the volcanic system characterized by processes evolving on disparate length and time scales.

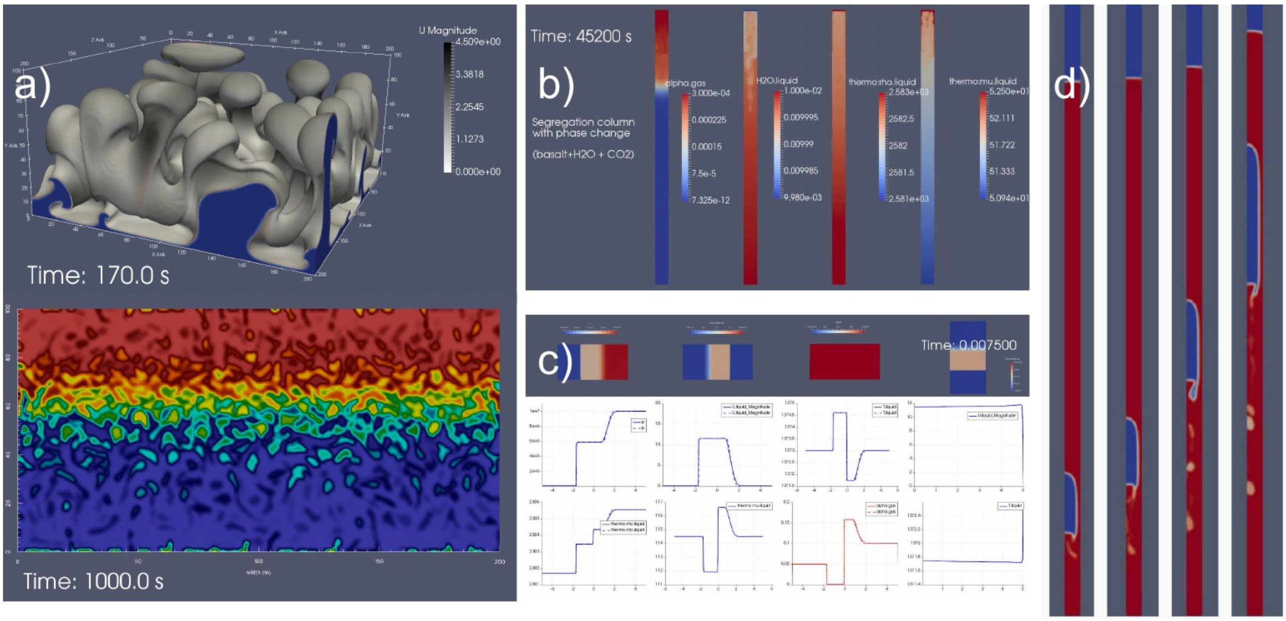

Fig.1 – Brief overview of MF applications relevant to magmatic systems:
a) Snapshots of 3D simulation of buoyancy-driven mixing due to the development of Rayleigh Taylor instabilities between two layers of magma with different densities. Initially an heavy layer (gas-free) is placed on top of a ligher one (with gas bubbles) in a box 200x100x200 m. After 1000s the overturning process is almost complete.
b) Simulation where the density difference driving the mixing is caused by the exsolution of gas bubbles (phase change). The intial setup is a column filled with a basalt oversaturated in volatiles (out of thermodynamic equilibrium) with a small fraction of gas bubbles. With time, the gas segregates and rises up into the column. After about ten hours gas bubbles concentrate at the top of the column due to segragation. In turn, the increased gas concentration causes the exsolution of volatiles that induces density differences that trigger gravitational instabilities and mixing dynamics.
c) Multiphase shock tube benchmark that is used to test the ability MF and OF multiphase solvers in resolving the propagation of shock waves and rapid decompression of magma (melt+gas) in closed volcanic conduit.
d) Space time evolution of a large gas bubble, a *slug*, rising in an open conduit. As the slug rises the nose accelerates due to volume expansion caused by decreasing hydrostatic pressure. Rapid ascent and bursting at magma air surface is responsible for repetitive explosive strombolian activity.

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Development of a High Performance Hydrological Model

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Keywords: GEOtop, hydrology, software engineering, Julia

GEOtop is an integrated hydrological model that simulates the heat and water budgets at and below the soil surface. Typical examples of its applications include flood and drought forecasting, water resource management, agricultural productivity forecasting and climate assessment studies. The latest version of GEOtop has been partially rewritten in C++ from C and its source code is available on GitHub with a GPL3 licence.

The development of this software spans over a decade and is the result of the layering of contributions from developers with different backgrounds and more emphasis on the scientific results than the code quality. Therefore, although being scientifically advanced, the codebase and documentation of this model suffer a big technological debt (something not uncommon among scientific software projects of this size) and the application has issues of performance and stability.

Therefore, in recent years there has been an effort to fix those issues, with the ultimate goal of ease further development, increase usability, ease the integration with other packages and pre- and post-processing tools and enhance its performance. In synthesis, the ongoing development of GEOtop is aimed at the development of both a high-productivity and high-performance hydrological model.

In particular, a new phase of development will be conducted approximately in the period spring-fall of 2020 within a MHPC thesis project (SISSA & ICTP), under the supervision of the cofinancing HPC-TRES sponsor Eurac Research.

Before the actual development can begin, the status of the project and its possible future developments have been discussed and are now submitted to the community to collect feedback and opinions. Up to now, the main proposals are:

1. continue the refactoring/reengineering of GEOtop to enhance the performance and stability of the software, more practically this would mean
   A) replace custom linear algebra routines with standard BLAS/LAPACK packages,
   B) simplifying the IO (for example, by removing useless dumps on disk),
   C) modularize the codebase,
   D) enable multithreading (e.g. in linear algebra and by parallelizing the energy/mass balance routines),
   E) profiling the code to do further optimizations;
2. standardize the pre- and post-processing within a Python/Julia library, which, for example, could encapsulate and manage the GEOtop app;

3. create a framework/library in Python/Julia for launching multiple instances of GEOtop and make ensemble analysis (e.g. for parameter space exploration, coupling with stochastic meteorological models or training neural nets).

Another possibility is a complete rewrite of GEOtop as a Python/Julia library (as opposed to a monolithic application). However, after careful consideration, this scenario has been considered unfeasible, unless the community would demonstrate a strong interest in this and be willing to provide some help.

On the other hand, running GEOtop on a multi-node architecture to do ensemble analysis seems to be a favourable possibility as it will enable GEOtop to both go into an HPC regime and produce results scientific interest unprecedented for this model.

In both regards, Julia is a particularly good candidate to work with. This general-purpose high-performance programming language has been recently developed at MIT with scientific/technical applications in mind. In particular, it has been designed to solve the two language problem, that is the issue, commonly found in the scientific computing environment, where one has to write software frontends in languages with more expressive power like Python or MatLab and backends in more performant languages like C/C++ or Fortran.

Indeed, Julia can reach performance comparable C while being more abstract and encouraging code reuse. This is possible thanks to both compiler technology advancements (specifically, Julia utilizes the compiler framework LLVM) and design choices. The most relevant among the latter is probably the dynamic multiple dispatch, which allows writing generic, extensible interfaces. The main difference of this kind of polymorphism, as opposed to single dispatch (common among other object-oriented programming languages), is the selection of the implementation of a polymorphic method (specialization) based on the type of all its arguments together and not separately.

Other useful features of the language are a built-in package manager, plenty of packages and built-in utilities for scientific computing (e.g. special functions, array broadcasting, etc.), a "no boilerplate" philosophy for integration with C and Fortran libraries, homoiconicity and native support for parallel and heterogeneous computing.

Acknowledgement

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Seismic and Electro-Magnetic wave modeling

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Keywords: Seismic, Electro-Magnetic, forward modeling, inversion, optimization

The modeling of seismic and electro-magnetic (EM) waves propagation is a complex and usually computationally-intensive task. The numerical codes used for the underlying computations are tools in constant evolution, mainly for two reasons, either to include more physical details or to improve their computational efficiency.

In some simplistic cases – usually where the geometry of the medium is simple - analytical solutions to the waves equations (either seismic and EM) can be found, however for more complex geometries the wavefields can be computed only through numerical solvers. The main costs of these numerical solvers can be separated into two categories: technical costs (computation time for a given problem, quantity of resources used – e.g. CPUs, Memory – complexity of the mathematical theory in the numerical schemes, ...) and human costs (code development time, code maintenance, end-user friendliness of the codes, …). While the geophysics researchers main interest lies within the practical applications of the modeling codes, they have a constant interest in keeping their modeling tools as efficient and easy to use, hence the need for recurrent (re-)engineering efforts.

The SEISLAB project had the goal to centralize the access to OGS' resources (e.g. seismic data), and simplify the workflow for all the tasks performed usually by several scientists by providing a unified access to both the data and the tools to process them. Part of the project was developing, optimizing, and parallelizing some pre-existing 2D and 3D seismic modeling serial codes (e.g. Carcione J.-M., 2007). Special attention was given to flexibility of use and efficiency through proper choice of FFT library, code optimization, adapted parallelization, and an upgrade of the boundary layers system. Finally, an additional care was given to providing a simple interface and tooling for preparing modeling runs, as well as providing synthetic outputs in consistent format with respect to the usual formats used in the processing and analysis of real seismic data.
All improvements allowed to compute synthetic datasets for two challenging studies in a reasonable time, only one (Zhu et al., 2019) being published at the present time.

The DILEMMA project aims at monitoring the river banks and levees structural integrity (for all rivers in Italy) through conductivity measurements using the DUALEM instrument (e.g. Saey et al., 2009). In order to improve the accuracy of the monitoring, an in-house inversion scheme is currently in development, using old EM modeling code (Sing et al., 2010) which had first to be ported to modern programming and flexibility standards. This inversion scheme intends to use a new strategy for minimizing the misfit function ('error' between measured data and synthetic data), allowing for more than only one optimisation algorithm at the same time. To do that, the HOPSPACK (Hybrid Optimization Parallel Search PACKage, Plantenga T.D., 2009) package is considered, since it allows naturally to use multiple search algorithms at the same time in a concurrent way, in order to converge faster towards the minimum of the function to minimize. Different options about the number and nature for the search algorithms are under consideration.

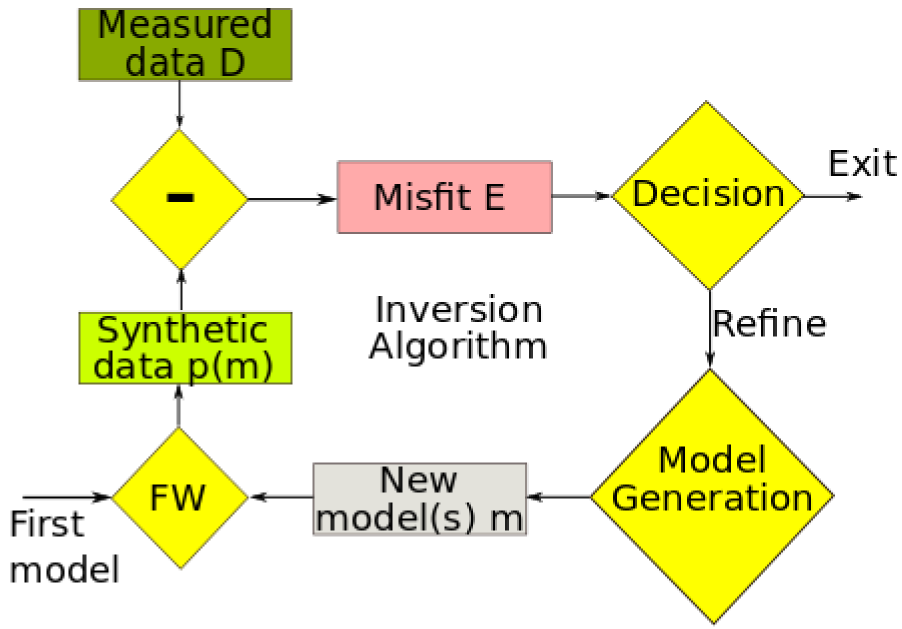

Fig.1 – Flow chart of an inversion algorithm; the type of modeling (producing the synthetic data) and the strategy (or in our case 'strategies') for the Model Generation defines the nature of the inversion algorithm.

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Imaging and numerical geophysics (ING)

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Keywords: geophysics, dark fiber, full wave inversion, seismic event detection

The field of geophysical imaging establishes an important branch of the underground studies. Since plenty of resources, such as gasses, oil, minerals and energy come from the core of the Earth can be found underground, it is necessary to carry out several studies to investigate and exploit its features. Nevertheless the underground it is also an hazard for humanity, in fact, monitoring of seismic events play a main role in our lives.

Obtaining an image of subsoil is still a difficult task to accomplish: there exist a lot of ways to look under the ground, but all of these are affected by high inaccuracy. Through the usage of several surveying techniques it is possible to have an idea of the underground profile using a lot of measurements (Fig 1.). These big datasets are managed by parallel computing techniques since to investigate these issues there is need of a huge computing power and a huge amount of memory. The full wave inversion method represents one of the most proficient tool to discover the underground, since it allows to reach high resolution in the field of ING. All the data coming from experiments are used by this method that provides underground matter properties. The main task is to handle memory resources in an efficient way to reach the best image resolution.

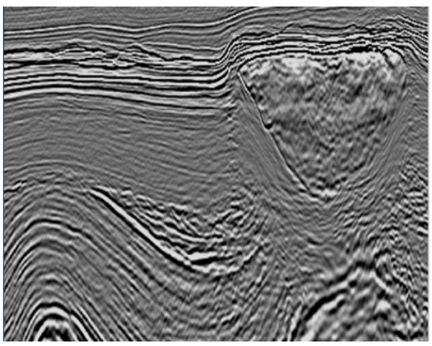

Fig.1 - Image of subsoil obtained with full wave inversion method.

This project is still under development, it can change purpose and shape, but it will belong to B10 research line of the HPC-TRES activity. In this sense, attention is given to the problem of seismic event detection. Monitoring of underground environment through dark fiber DAS is a new way to create a distributed platform of sensors built in the underground that provide near-surface soil properties and earthquake seismology. Moreover, it provides a huge amount of collected data that only parallel computing techniques can perform.

Usually cables are located along underground corridors, as roads, rail connections and oil pipelines, so they are affected by a rich component in ambient seismic noise, that can be extracted releasing space to significant measurements(Fig 2.).
Through the analysis of these seismic data is it possible to obtain information of the seismic and hydrological state, in particular during earthquakes. Limit of this method is data retrieval, because they belong to the telecommunication companies.
Future developments will contribute to the reshaping of this project, but the focus on the usage of HPC techniques to investigate the underground environment will be maintained.

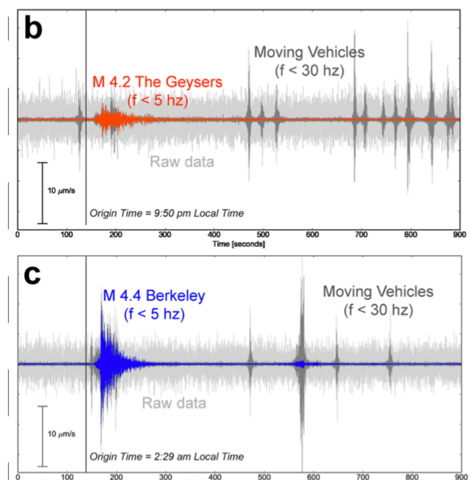

Fig.2 - Raw and lowpass filtered DAS strain-rate waveforms for these events averaged over 100 m (50 channels) at the yellow circle position shown in (a) (channel 4975 +/− 50 channels). Note the similarity between seismic and non-seismic signal amplitudes and the differences in frequency content

Acknowledgement

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Paleo-modelling of Antarctic ice sheet: preliminary results and challenges

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Keywords: ice sheet modelling, paleoclimate, Antarctica

Ice sheets are continental-size ice body that flows because of the lope of subglacial topography, of the slope of the ice sheet margins, and because of internal deformation of the ice. The ice motion is described by the so-called Navier-Stokes equation, that link horizontal and vertical advection of the ice to temperature. Internal ice temperature is described by the temperature diffusion equation which takes as boundary conditions atmospheric surface air temperature, geothermal heat fluxes coming from the Earth's core and mantle, that both diffuses through the ice column. Mass balance of the ice sheet is determined by how much snowfall reach Antarctica, how much calving occurs at the front of floating terminations of the ice sheet (ice shelves) and how much sub-ice shelf melting occurs due to ocean warming. The ice sheet also have a particular rheology, the deformation of the ice crystal determines the velocity of the flow by determining the isotropy (crystals oriented in the same direction) or anisotropy (no preferential direction in ice crystals) of the ice crystals. Deformations follows the 3D-mechanical tensor of stresses and are related to the Navier-Stokes equation through the Glenn-flow law, describing the relationship between shear stresses of the ice and its viscosity (which depends on time and ice temperature).

Ice flow happens on a very long-time scale, because deformation of the ice is very slow (cm/year) and because of the basal friction when flowing on a hard-grounded bed. However, along the coast, when the ice sheet reaches ocean, it starts floating, no more friction occurs and ice flow accelerates to a speed up to several km/year. Because of the slow temperature diffusion through the ice column, the thermal inertia of an ice sheet is very long, of the order of several millenia to a couple of tens of millenia. This implies that the climate memory of an ice sheet is also as long as its thermal inertia. As a result of this caveat, and as for any climatic model requiring spin-up of its thermodynamics, ice sheet models require long-term realistic spin-up of about one to two glacial cycles, i.e. circa 200,000 years, before attempting any projection of the future. Other more rapid technics have been developed but because projections show that Antarctic would melt even more in the net centuries, beyond 2100, realistic long-term initialisation of ice velocities is needed instead of quick short-term spin-up.

On MARCONI and then GALILEO supercomputers, the Parallel Ice Sheet Model (Wincklemann et al, 2011, Martin et al., 2011) was installed and compiled. This model offers a good scalability of ice sheet dynamics and allow to reach resolution up to 5 km over regional domains. Long-term spin-up at 15 km of resolutions are running using 4 nodes (144 CPUs) and allow to run this sin-up in three days. So far, the spin-up do not result in a satisfactorily Antarctic ice sheet geometry for present-day, i.e. some of its margins are located too much inland, or some other sectors are too expanded compared to present-day configuration. Tuning of sub-shelf melting due to ocean warming, calving criterion and modulation of ice sheet velocities are necessary to produce a realistic present-day configuration. Computing hours are provided by ISCRAC-ANTCAL0 for the moment. A full ensemble of about 100 to 200 simulations is necessary to obtain a set of parameters leading to a good initial state of the ice sheet. Work in progress.

Acknowledgement

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Numerical methods for Full Waveform Inversion. Analysis and implementation

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Keywords: Full Waveform Inversion, numerical optimization

A standard method to recover quantitative information on the Earth subsurface is based on travel-time tomography. From the measurement of the distance between the sources and the receivers, and the recording of wave first-arrival times, an estimation of the wave velocity field can be computed. This method has proven to be useful in many cases, especially when the subsurface geometry keeps simple. In presence of complex structures, the quality of the velocity estimation provided by the reflection tomography method may be degraded.
The Full Waveform Inversion (FWI) approach has been designed to overcome these difficulties. This technique is used for estimating a high-resolution model of the subsurface and can be employed for various targets, as for instance the localisation of water and natural resources such as oil and gas, the storage and reservoir monitoring, and seismic risk prevention.
In a seismic acquisition the seismic waves, created by a controlled source, propagate through the subsurface. Some of them return to the surface as refractions or reflections from geological boundaries within the subsurface. The arrival times and the amplitudes of the waves at different offsets from the source are measured by a set of receivers, distributed on the surface. The data measured by the seismogram, that is the set of all the seismic traces relative to the same shot, are so used to reconstruct the geological subsurface model, given by wave velocity and layer's depth.
Conventional FWI consists in minimizing, with respect to the Earth model, a misfit function which measures the distance between the predicted and the observed data trace. This leads to solving a strongly nonlinear and potentially large scale least-squares problem.
One problem with current implementations of FWI is the presence of local minima in the objective function produced by cycle skipping. Adaptive waveform inversion (AWI) reformulates FWI using adaptive matching filters and it claims to overcome cycle skipping during waveform inversion. In contrast to FWI, AWI does not seek to minimize the difference between the observed and predicted data set directly. Instead, it proceeds by finding a suite of data-adaptive matching filters, depending on the observed and the predicted data, which transform one of these data sets into the other. The waveform inversion problem can therefore be setup to minimize not the data misfit directly, but instead the misfit between the filters matching the two data sets and the identity filter.
Gradient based numerical method's, such as the method of steepest descent, can be used to solve the minimization problem. By this method, to find a minimum of a function one takes steps proportional to the negative of the gradient of the function at the current point. This setting requires the gradient evaluation at each iteration. To avoid this, and so to reduce computational costs, one idea is to use an approximation of the gradient provided by some numerical techniques already used for other problems.

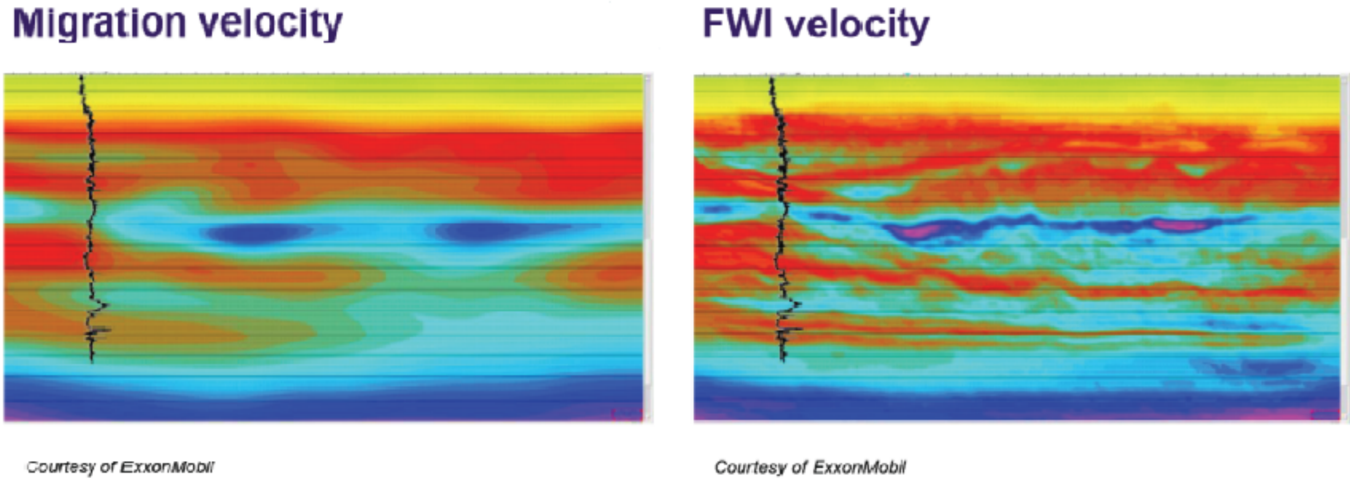

Fig.1 – Vertical estimated section of the Earth (from Tariq Alkhalifah, EAGE Course, 2017).

Acknowledgement

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My journey from Academia to Industry

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Keywords: recommendations, wine, app, academia, industry

At first glance, **academia** and **industry** can seem two worlds far apart, and academic training might seem ill-suited to careers in private companies. Here I would like to share my experience in the transition from academia to industry and show that my scientific background has proven to be really useful in my current career.

As a Ph.D. student I was studying how the **diversity of plankton** could impact the mechanism of **carbon sequestration** in the deep ocean. This is an important **biologically** mediated phenomenon, which impacts **climate** since the ocean exchanges carbon dioxide with the atmosphere at the surface. To face this challenge, I built a **biogeochemical model** from scratch, to get some insights on these complex interactions and obtain estimates of biogeochemical fluxes mediated by plankton. Shortly before my graduation, I had a model capable of catching complex features of the water column, as the **deep chlorophyll maximum**.

After the Ph.D. I decided to move to a private company and work as a **developer** in the Research and Development group: currently we are trying to build a **wine application** for **mobile devices**; one might wonder why an app about wines? Because actually they offer exciting challenges!

Wine has an incredible diversity: there exist over **10 000 different varieties** of wine grapes worldwide, and each can be processed in a hundred thousand unique ways. That is why trying to **recommend** a wine to somebody poses interesting and difficult challenges. What are the key properties of a wine? Sommeliers have been dedicating their lives to craft wine's flavour profiles, so how can we discover these properties in advance, and try to represent them mathematically? That is what we are trying to accomplish: to build a **recommender system** for wines, inside our wine application so that users can get wine **suggestions** and then have a guided **tasting experience**.

Recommender systems are a subclass of information filtering systems that seek to **predict** the **rate** or **preference** a user would give to an item, based on user's interactions. We all have everyday experience on recommender systems: when we watch a movie or TV series online, when we purchase something, or even when we make friends on social media, there is "something" which suggests to us new movies, products, or people we should know based on our behaviour and interactions: that is the recommender system!

A recommender system is a technological and algorithmic challenge *per se*, and there are in principle several different algorithms that can be implemented to obtain a reliable one. We chose a rather simple but effective approach: it consists in **reducing the dimensionality** of the problem and then apply a **cluster analysis** on the wines contained in our database; these are represented as numerical vectors, and have more than 200 coordinates, that is why we need to reduce the dimensions. After that, cluster analysis is needed to understand which wines are similar in **tasting, smell, and visual properties**.

In Figure 1 we show a screenshot of the application with the detail of a wine, together with a plot of our wines projected in 2-D and clustered.

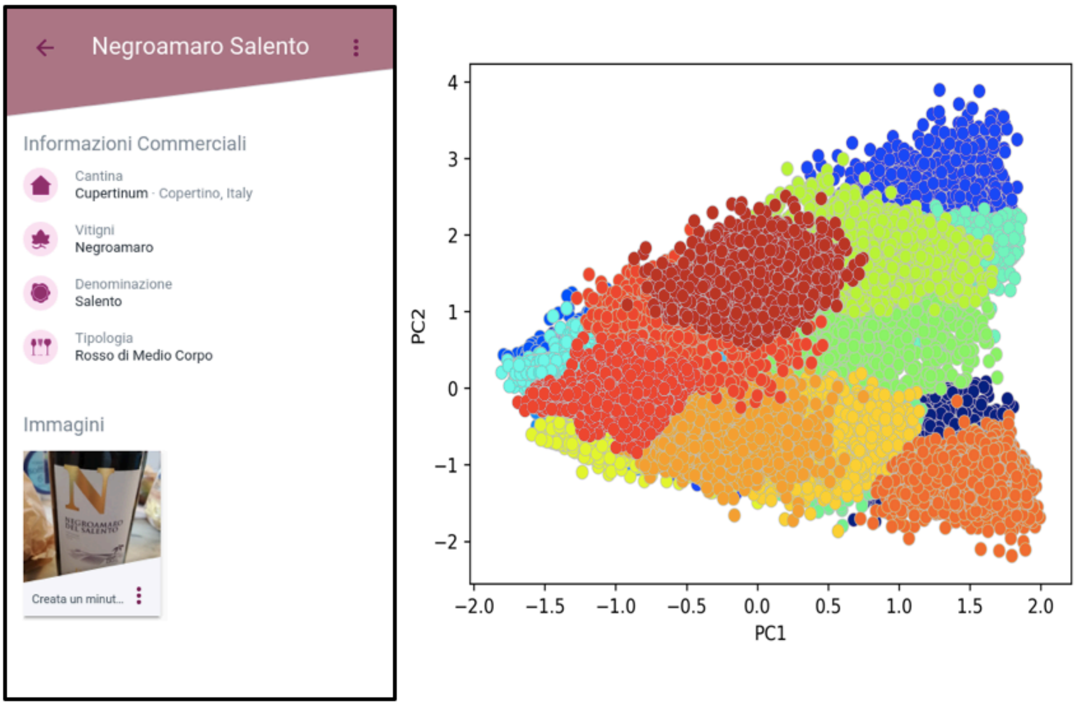

Fig.1 – Left: screenshot from the wine application, with an example wine's commercial info and label picture. Right: plot of the wine clusters obtained with dimensionality reduction + cluster analysis on our data.

It may seem that my present work and the Ph.D. experience are completely unlinked. Instead, many **skills** that I have learnt during my studies are currently being used in my everyday work, for example **critical thinking**, **technical writing**, or the ability to work with **data** and make decisions based on it.
In conclusion, when thinking about possible careers in private companies, PhDs have already many of the valuable abilities that are wanted.

Acknowledgements

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We acknowledge the CINECA award under the ISCRA initiative, for the availability of high performance computing resources and support (IscraC "HYPER").
The results of the second part of this document are fruit of the teamwork by Esteco's Research and Development Group.

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MITgcm(BFM) focus on marine biogeochemistry: emerging scales of variability

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Keywords: modeling, ecosystem, scales, Mediterranean Sea, Northern Adriatic Sea

Oceans host a lot of non-linear and inter-connected processes, involving physics, chemistry and biology, on a wide range of spatial and temporal scales. In particular, marine biogeochemistry has impacts on the ecosystem function and services (e.g. the fishing) from the regional scales up to the global scale, where the biogeochemical cycles (e.g. the carbon cycle) contribute to determine the environmental state and the climate of the whole planet.
Coupled physical-biogeochemical models are useful tools to describe such complex systems, providing complementary information to observational systems (e.g. floats, cruise campaigns, remote sensing). Numerical models typically describe biogeochemical processes in the ocean from tens of meters and hourly frequencies to the planetary scale and hundreds of years of simulation, respectively.

The MITgcm-BFM model, obtained coupling the General Circulation Model developed by the Massachusetts Institute of Technology and the Biogeochemical Flux Model, developed by a consortium of scientific institutes, can be implemented to describe marine processes on this whole range of scales. In particular, we configured it to describe the dynamics of the marine ecosystem at the basin scale, i.e. on the Mediterranean Sea, and on a coastal region, i.e. the Northern Adriatic Sea. In both cases the coupling was online (Cossarini et al. 2017) with the MITgcm acting as the master model, which solves the Navier-Stokes equations and provides physical dynamics and transport, and the BFM acting as a library of biogeochemical reactions, which solves ordinary differential equations for the mass fluxes of 51 constituents and nutrients, in the water dissolved phase, in the plankton and in the detritus compartment.

In the Mediterranean simulation (Di Biagio et al. 2019), the grid had a horizontal resolution of 1/12° (about 7 km) and 75 unevenly spaced vertical levels, the atmospheric forcing came from 3-hourly ERA-Interim fields and the riverine input frequency was monthly. The main variables describing the marine ecosystems had a daily output frequency, for a total of 8 terabyte of produced data for the 1979-2012 simulated period. The adopted spatial resolution allowed to characterise the biogeochemical gradients on the sub-domain scale down to the mesoscale (i.e. tens of kilometers), related to the productivity of the basin both at surface and along the vertical direction (e.g. evaluated from the Deep Chlorophyll Maximum, DCM). On the other hand, the daily frequency output of the main ecosystem variables along the multi-decadal period allowed to characterise the temporal variability of the ecosystem state from the sub-weekly to the inter-annual scale, using a set of novel statistical metrics. In particular, we found a southward decreasing gradient across the basin for both the seasonal and the sub-weekly variability (Fig. 1) for all the main ecosystem variables.

In the coastal application, MITgcm-BFM was integrated with the national dataset of biogeochemical variables provided by ISPRA, including nutrients and chlorophyll from coastal stations and nutrients measured at urban waste water treatment plants (UWTTP), within the CADEAU project (Silvestri et al. 2018). CADEAU provides a downstream CMEMS (i.e. Copernicus Marine Environment Monitoring Service) product focused on the monitoring of the

environmental status of the Northern Adriatic Sea in the last decade, with yearly update until 2020.
The horizontal resolution of the coupled model in this case was 1/128° (about 700 m). The model was driven by the downscaling of the daily Mediterranean CMEMS hydrodynamics and biogeochemistry at the southern boundary, by an atmospheric forcing coming from hourly COSMO-LAMI fields and daily riverine inputs for the major rivers of the area (Po, Timavo, Isonzo). In this case, with a total amount of 1.5 terabyte of produced data, the model was able to characterise processes down the scale of few kilometers. For example, we estimated the influence area of the plumes came out from the UWWTP of the Chioggia municipality on the neighbouring bathing waters and aquaculture areas. To do this, we simulated the dynamics of 12 tracers, decaying with a first order law in dependence of temperature, salinity and irradiance conditions (Chan et al. 2013) and thus used as a proxy of faecal bacteria (e.g. Escherichia Coli), that were released at UWWTP sites in the Chioggia municipality.

The pre-operational version of MITgcm-BFM for the 36-hourly forecast on the Northern Adriatic Sea, with atmospheric forcing from ALADIN model, is currently running at the CINECA supercomputing centre (http:/medeaf.inogs.it).

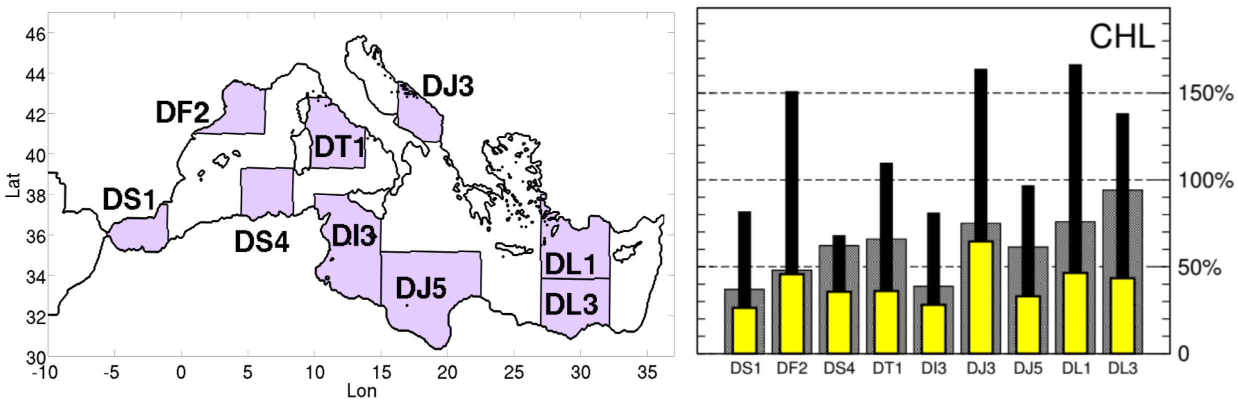

Fig.1 - Statistical estimate for the seasonal and the sub-weekly variability (black and yellow bars of the right plot, respectively) for the modeled surface chlorophyll concentration, spatially averaged on the Mediterranean sub-domains (left plot), following the subdivision by Manca et al 2004. Grey bars in the right plot represent the inter-annual modulation of the seasonal variability. Please refer to Di Biagio et al. 2019 for the definitions of the statistical metrics and further details.

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award number 2016-04 and by 2016-2018 CADEAU UserUptake CMEMS project. We acknowledge the CINECA award under the ISCRA initiative, for the availability of high performance computing resources and support (IscraC "IsC34_BIOMEDCO", "IsC41_BIOMEDXT", "IsC45_BLOMEDXT", "IsC55_CADRI").

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The regional earth system model RegCM-ES: state and perspectives.

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Keywords: regional earth system model, hydrological cycle, climate change

Thanks to the development of the regional earth system model RegCM-ES (Sitz et al., 2017), it has been possible to take into account phenomena that are driven by the interaction of two fundamental climatic components of the Earth System: the atmosphere and the ocean. As well known in the literature, the climate variability of some atmospheric and oceanic phenomena can be reproduced correctly through the use of a model only if we consider the interactions between these two components. In some cases, the contribution of factors not immediately linked to these phenomena, can play an important role in the interactive system.

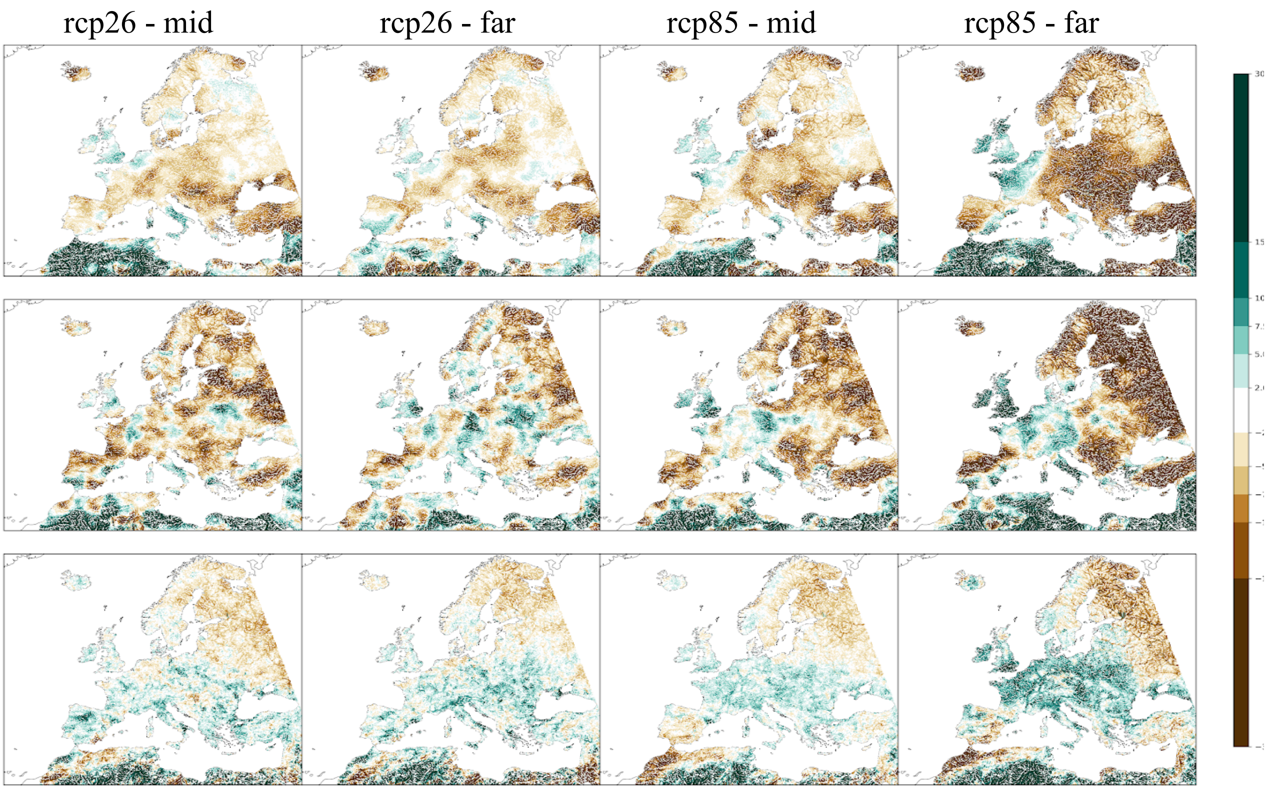

Fig.1 - Relative changes of multi-model ensemble mean of Q100 index for different scenarios and time slices. In the top panels are shown the CMIP5 models for the mid and far future and for the rcp26 and rcp85 scenarios in comparison to the reference period. In the middle panels are shown the CMIP6 models for the mid and far future and for the rcp26 and rcp85 scenarios in comparison to the reference period. In the top panels are shown the CMIP5 models for the mid and far future and for the ssp126 and ssp585 scenarios in comparison to the reference period. In the bottom panels are shown the CORDEX models for the mid and far future and for the rcp26 and rcp85 scenarios in comparison to the reference period.

It would be enough to think how it is relevant the contribution, of the huge amount of freshwater discharge flowing into the Bay of Bengal, on the formation of a barrier layer to the ocean mixing.

This barrier layer makes the ocean more reactive to the atmospheric variability modulating the feedback between the two components. Whit this in mind, an hydrological model is essential to take into account this contribution but it would be not enough if we did not take into account also the non-negligible effects, like the stirring of the wind, that would nullify this contribution. Let's think, for example, how an overestimation of the winds could have a destructive effect on the formation of the oceanic barrier layer. An unrealistic representation of the ocean waves can be one of the motivations of the excessive mixing, and a new component capable to simulate them, could be decisive in this regard (Di Sante et al., 2019). In a perspective of increasing availability of computational resources, could be interesting the possibility of using RegCM-ES with convection permitting resolutions. In fact, ongoing studies show how the contribution of the air-sea feedback increases with the horizontal and vertical resolution of the model components.
Recently, more focus has been dedicated to a number of extreme phenomena that, in a climate change contest, could represent a serious threaten to the regional health and economy of some areas of our planet. One of these phenomena are the flooding; a warmer atmosphere is able to contain a greater water quantity and it is legitimate to think how, with the increase of global temperatures, we could face an increase of extreme precipitations and flooding. The parallelized version of the distributed hydrological model (CHyM) has been successfully been coupled offline to a great number of regional and global coordinate climate simulations (CORDEX, CMIP5 and CMIP6) and applied to simulate the effects of the global warming on the floods risk over the European region. (Di Sante and Coppola, 2019).

Acknowledgement

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A breakdown of the link between Arctic and North Atlantic Oscillations in warm climate projections

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Keywords: North Atlantic Oscillation, Arctic Oscillation.

The North Atlantic Oscillation (NAO) and the Arctic Oscillation (AO) are climate variability modes linked to a large fraction of temperature and precipitation variability in the mid-latitudes of the Northern hemisphere. In this study, we use both reanalysis data and model historical and warmer climate simulations to show that the relation between the two oscillations may change dramatically in a different climate. In the current climate, these two climate modes are highly correlated, and they are both strongly influenced by downward propagation of stratospheric anomalies into the troposphere. When considering a warmer climate scenario (RCP8.5 in the XXIII century), the correlation between NAO and AO drops significantly, revealing that they become two separate modes of variability. The stratosphere remains an important precursor for NAO, while the AO consistently precede stratospheric anomalies. The analysis suggests that these changes are owed to land-sea thermal contrast intensification in the Pacific region, which becomes more favourable for storm variability.

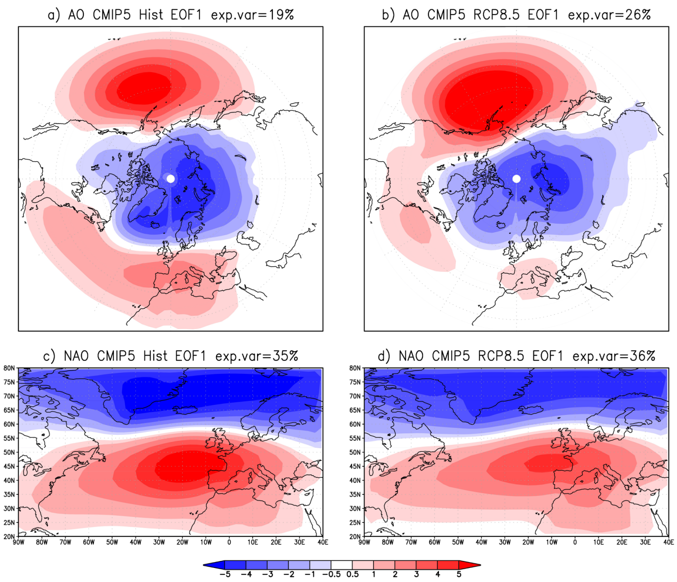

Fig.1 - Multi-model average of the leading EOF mode for wintertime (DJF) sea level pressure. a) & b) are (AO) for Historical and RCP8.5. c) & d) are (NAO) for Historical and RCP8.5.

Acknowledgement

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New visualization tools for the Mediterranean Sea biogeochemical model (MedBFM)

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Keywords: data, visualization, tools, 3D, ParaView

Most people have an idea of the ocean as a surface, however, the third dimension is indeed extremely important. Sunlight penetration or vertical transport processes are key to biological dynamics. The OGSTM-BFM, i.e., OGS Tracer Model – Biogeochemical Flux Model (Vichi et al., 2015) code uses highly optimized 3D transport reactions non-linear PDE to model biogeochemical processes on the Mediterranean Sea. Therefore, efficient data analysis and visualization is crucial to comprehend the dynamics of the sea, for example to understand the spatial variability of relevant magnitudes such as chlorophyll (Lazzari, 2012) and phosphate (Lazzari, 2016) concentration.

ParaView (Ahrens, 2005) is an open-source, powerful data analysis and visualization tool built on top of the VTK library (Schroeder, 2000). It has been designed to analyze extremely large datasets using distributed memory computing resources, hence, it is ideal to run on supercomputers. Data exploration can be performed either interactively in 3D or programmatically using its python interface. Moreover, it can be easily extended by means of plug-ins written in either Python or C++. The present work aims to extend the capabilities of ParaView to enable the visualization of biogeochemical model outputs for the Mediterranean Sea. These set of tools are the "OGS ParaView Suite", which is the evolution of previous tools developed by the author and Cosimo Livi (Livi, 2017), and can be used to analyze the data from OGSTM-BFM and/or Copernicus Marine service.

The workflow for bringing biogeochemical data from OGSTM-BFM to ParaView is the following: firstly, the *OGS2Paraview* script is used to generate mesh and master files. These files are used by ParaView to relate the variables and the timesteps and to generate the rectilinear grid. Then, the reader plugin allows to seamlessly open the dataset on ParaView. Once in the application, a number of tools have been developed to work with various masks, for example, to select sub-basins or to cut the mesh. Other tools have been developed to compute gradients and vorticial structures, as well as, spatial and time statistics. These data can be visualized in three dimensions and exported back to NetCDF or Python Numpy format. The "OGS ParaView Suite" also allows to produce two dimensional outputs in the form of two-dimensional surface maps, depth profiles, spaghetti and Hovmoeller plots.

Another of ParaView's capabilities is to be able to work in a client/server configuration, allowing to have the data in a powerful machine (server) and using the local machine (client) just for visualization. The client/server configuration is advantageous as the data (usually in the range of terabytes of information) does not need to be transferred to the local machine. Moreover, in some circumstances, the rendering is also done in the server, thus enabling the use of accelerators such as GPUs.

In fact, developing on an ever evolving platform such as ParaView provides a number of features that are worth exploring, e.g., volumetric rendering (Fig. 1). Thanks to the client/server approach, the full power of ParaView can be used without penalties for the user's computer. In addition, Blender, a tool widely used by graphic artists, can also interface with ParaView and VTK and can provide interesting features in the future.

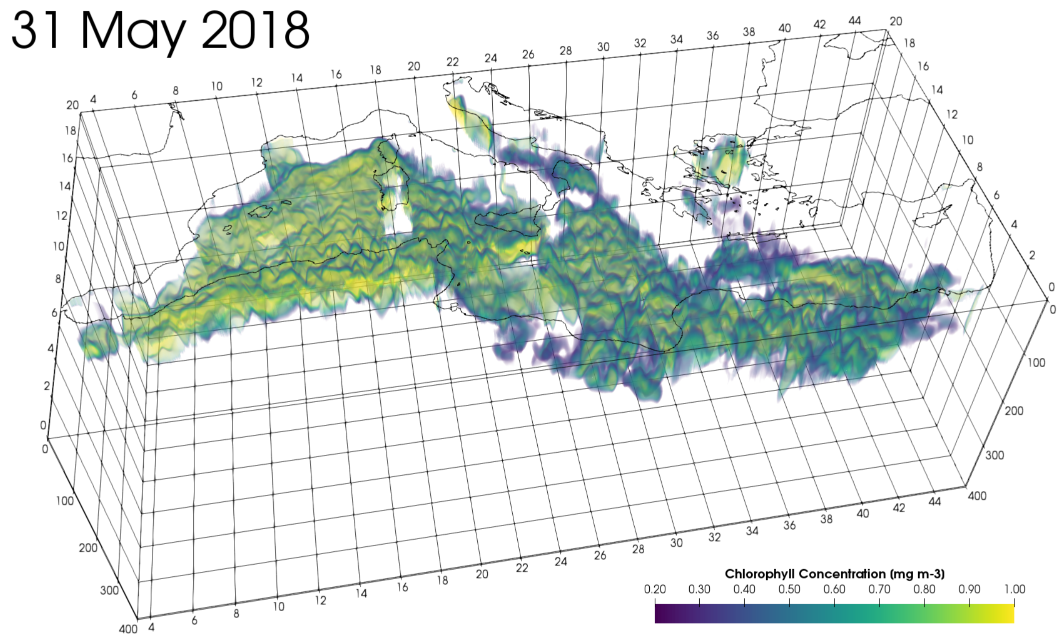

Fig.1 – Volumetric visualization of the chlorophyll concentration on the Mediterranean Sea using the nVIDIA IndeX rendering capabilities of ParaView. Credits: "Generated with E.U. Copernicus Marine Service Information".

Acknowledgement

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User vs Exascale

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Keywords: HPC, Exascale

Cineca was established in 1969 to host cutting hedge supercomputer systems, together with the provision of access and support services to the Italian national scientific community. Since then the world of information technologies has been revolutionized many times, and the computer power has been improved several orders of magnitude, and Cineca was (has always been) able to offer always the best in class technologies and related services, allowing Italian (and now European) researches to be highly competitive worldwide.

To maintains high the european scientific competitiveness, the European Union set up an ambitious program for HPC and HPDA. In March 2017 in Rome, a number of EU countries, including Italy, signed the EuroHPC [2] agreement to establish a new joint undertaking organization to buy and deploy two pre-exascale and two exascale systems to be deployed in Europe in the timeframe 2021-2023. Italy candidates Cineca to host one of these system (Leonardo HPC) that, when deployed, could potentially be the most powerful system in the world. In USA, The Exascale Computing Project[3], likes EuroHPC, 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, and for this reason all the largest American chip manufacturers are focused on producing processors to reach this target in time, developing new technologies.

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 goal, concisely laid out in the following chart, is to ensure the Europe Union isn't dependent on anyone else for its exascale processor needs.

The performance of the most widely used architectural designs are slowing down (from one generation to the next) and its growth will be no longer exponential. The consequence of reaching this limit is the renewed interest in new architectural designs (post von Neumann), and new devices that can drastically change the rules of the game and allow the realization of devices with superior performance thanks to a different organization of available resources. All this has a price: having to rethink the applications according to the new architectures, in a process commonly known as co-design. In this way, new solutions can be created that present a closer relationship between the architecture and the application, in a process of verticalization that results in having architectures, which at various levels can be specialized for a purpose.

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[2] https://eurohpc-ju.europa.eu/

[3] https://exascaleproject.org/exascale-computing-project/

Hydroacoustic models for environmental applications

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Keywords: Computational Fluid Mechanics, Ffowcs-Williams Hawkings, Environment, OpenFOAM

In recent years the interest in the hydroacoustic field is growing, driven by the strong impact of the human activity on the environment. A lot of work was done to evaluate the effects of noise pollution on human beings, typically on land, but much less attention was paid to the effects on the marine environment. It is necessary to establish new methodologies to address the effect of the noise source in the marine environment like ships, oil survey, oil extraction, etc.

The main objective of this research is to evaluate the acoustic field generated by a complex source in motion submerged in a fluid. Among the existing methods availed to predict the acoustic field a hybrid method will be used. This method allows decoupling the fluid dynamic problem from the acoustic problem. Since to evaluate a noise source, firstly a numerical simulation of the fluid flow is carried out, then using an acoustic model, like the Ffowcs-Williams Hawkings [1], then the far-field acoustic field generated is recovered. Large Eddy Simulation is used to obtain an accurate fluid flow field. Capabilities on performing large numerical simulation, that will require HPC resources, will be developed mainly on the OpenFOAM framework [2].

This method is been already used to evaluate simple bodies in a uniform current [3] and also a more complex noise source, like a propeller [4]. The first study shows how the different shapes of the body affect the generation of the hydroacoustic noise. In particular, the ratio between the strength of the linear and non-linear terms of the FW-H equations is investigated. The second study shows how the turbulent wake generated by a propeller is a significant noise source, due to the presence of persistent vortex.

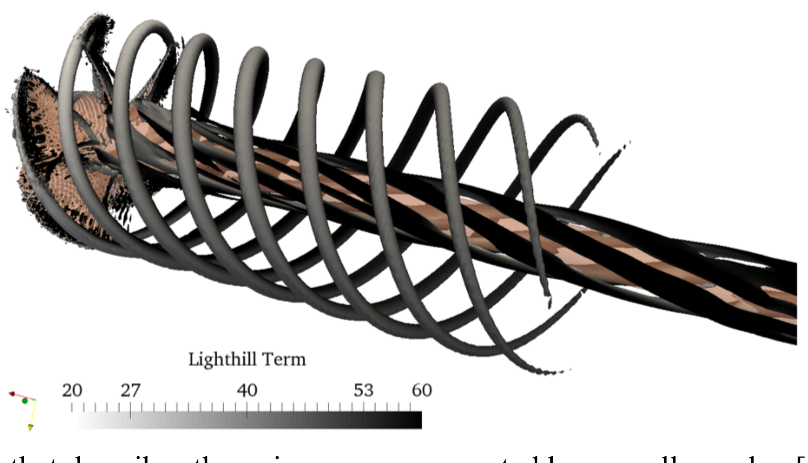

Fig 1. Lighthill term, that describes the noise source, generated by propeller wake. [5]

The main limit of the FW-H equations derives from the use of the Green's function, which allows obtaining a solution only for unbounded uniform acoustic medium. So, the future works are to understand and find a solution to this limitation. To ensure that the correct interaction between the environment and the noise source is evaluated. The main two problems that are going to be addressed are the presence of a boundary wall, like the seabed, and the presence of passive or active scalar in the flow, like the temperature.

Acknowledgement

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(Extreme) Synoptic patterns and biogeochemical dynamics in the Mediterranean Sea

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Keywords: Mediterranean Sea, Large-scale atmospheric circulation patterns, nutrients, mixed layer depth, dissolved oxygen, heat waves, cyclones

The Mediterranean Sea region is located in a transition zone between two different climate regimes (subtropical and mid-latitude). It is characterized by a complex land-sea distribution which affects deeply the atmospheric and oceanic flows and by a high density of population, industrial and touristic settlements which make the region particularly sensitive to extreme events, which are projected to increase in frequency in the area as a consequence of climate change.

Ocean and atmospheric variability over the area have been often associated with the state of the four modes of Northern Hemisphere modes of variability such NAO, EA, EA/WR and SCAN. These large-scale circulation patterns (LACPs) are known to influence heat fluxes and wind stress fields over the Mediterranean Sea and through them the mixed layer depth dynamics.
On the other hand limiting nutrients (Phosphate and Nitrate) distribution in the convective areas of the Mediterranean Sea is strongly linked to mixed layer depth dynamics. Thus, as LACPs are known to influence heat fluxes and wind stress fields over basin, it is interesting to investigate at which extent LACP may influence the nutrients concentration in the basin and if it is possible to quantify this influence.

To answer these questions, we used the historical timeseries of NAO, EA, EA/WR and SCAN indexes and 2D fields of total heat fluxes, wind stress, mixed layer depth, and 3D fields of PO4 and NO3 extracted from a simulation which covers the period January 1961-December 1999 and built using the offline coupling of NEMOMED8-OGSTM/BFM (Reale et al.,2019, in review).

Our work shows that changes in LACP over the Mediterranean region may affect the nutrient concentration in the main convective areas of the basin. More specifically the influence of LACP on long term nutrients variability is limited to the Gulf of Lions for PO4 and NO3 in the case of EA and for PO4 in the case of NAO patterns in the Aegean Sea and Rhodes Gyre area. Long-term variability of NO3 in the sub-basins of Eastern Mediterranean seems to be more correlated with river supply than large atmospheric circulation patterns.

Currently further analysis is carrying out on the impacts of the extreme synoptic patterns as heat waves and cyclones on dissolved oxygen and nutrients distributions in the convective areas of the basin. More specifically a signature of the heat waves of summer 2003 has been observed on the dissolved oxygen in the upper layer of the basin (first 25 m) and along the water column in the Southern Adriatic (fig.1 a). Still a signature of the passage of intense cyclones in the Strait of Sicily has been observed in the upwelling system along the Sicilian coastline (fig.1b).

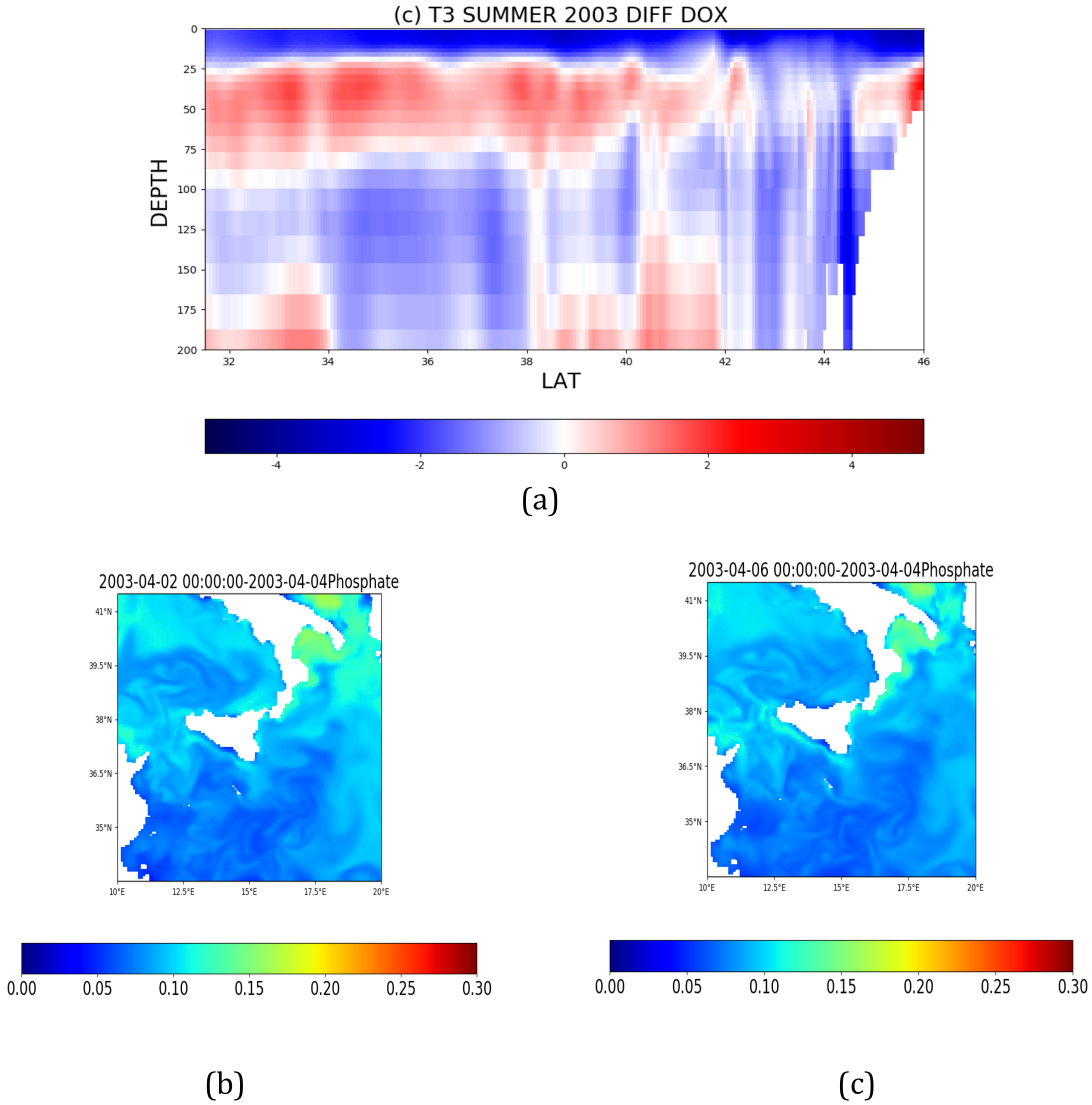

Fig.1 - (a) Dissolved oxygen anomaly (in mmol/m^3) during the summer 2003 along the Ionian-Adriatic Sea transect; distribution of the phosphate in the Sicily strait before (b) and after (c) the passage of a strong cyclone.

Acknowledgement

The research reported in this work was supported by OGS and CINECA under HPC-TRES program award number 2015-07. We acknowledge the CINECA award under the ISCRA initiative, for the availability of high performance computing resources and support (IscraC “LEPRE”,”ADDIO”,”TRICYCLO” and “DyBIO”).

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Calculation of Damage maps for seismic scenarios in North-Eastern Italy

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Keywords: Seismic damage assessment, seismic scenarios, modeling strategy, uncertainty

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, a limited number of damage and risk assessment exists for North-Eastern Italy, mostly based on probabilistic seismic hazard assessment and the use of vulnerability matrices (Bernardini et al., 2007) or Probit curves (Grimaz, 2009; Grimaz and Malisan, 2018).

We developed a damage assessment model that allows to estimate expected impacts on buildings and population for a given ground motion scenario. Damage calculations are performed with the OpenQuake program (Silva et al., 2014). The damage assessment model is combined with the USGS ShakeMaps that provides the ground motion estimates (Silva and Horspool, 2019). The parallel version of Openquake is not configured to work on an HPC-cluster as it makes use of a specific task queue service (Celery) which does not fit in a multiuser computing environment. However, it still supports process-based parallelism on single nodes. Thus, we developed a wrapper that allows to run multiple OpenQuake instances on the Galileo cluster at CINECA. The wrapper allows to specify the configuration parameters (e.g. queue type, output folder, input files, etc.) and to launch a number of independent realizations of the damage assessment model, initialized with a set of input parameters. Each run is then sent to a specific node, where it is locally parallelized. Note that the nodes calculation is performed independently and does not require any synchronization.

A Monte Carlo approach is used to sample the parameter space, creating an independent calculation run for each realization. In particular, after having reviewed the state-of-the-art, we decided to focus our analysis on building fragility. Despite of the relevance of this aspect, there are very few attempts of including the uncertainty of fragility curves in the damage assessment procedure (Bradley, 2010). We have been selecting the best-performing fragility curves for each building typology by running the damage assessment model for the Friuli 1976 earthquake, and comparing it with real damage data collected at the time. Each fragility curve has an associated uncertainty, that will be taken into account for the initialization of the damage assessment calculation. The input parameters will be stored and managed by the configuration files, organized in a hierarchical manner.

The modeling strategy proposed hereby (Fig.1) will allow to produce damage maps for specific scenarios, and to explore the uncertainty and its propagation on the resulting damage assessment. Further work will be focused on three aspects: performing a sensitivity analysis on the results, applying this methodology to specific scenarios and improving the visualization of the results.

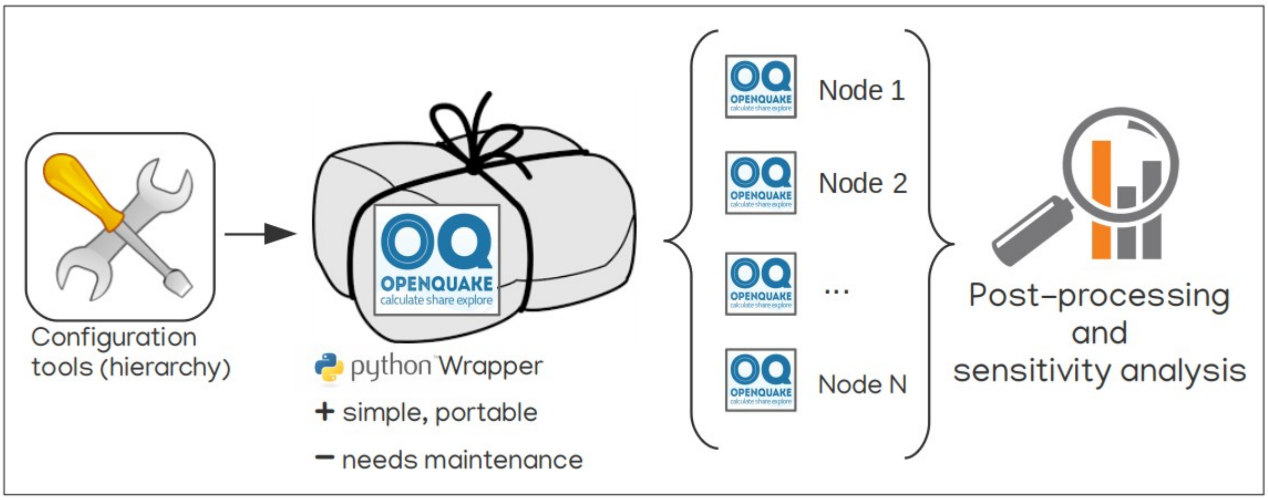

Fig.1: The modeling strategy workflow: input parameters are set through the configuration tools; the wrapper initializes the model and distributes the calculation at each node; finally, the post-processing is performed.

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The research reported in this work was supported by OGS and CINECA under HPC-TRES program award number 2019-03. We acknowledge the CINECA award under the ISCRA initiative, for the availability of high performance computing resources and support (IscraC "HYPER").

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Gravity data reduction and inverse modelling in compressional and extensional geodynamic settings

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Keywords: gravity data, inverse modelling, geodynamics

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 needs to recover all the data, arrange them in a coherent and usable database.

Gravity measurements are used in geophysics to point out subsurface bodies and density anomalies within the Earth. By removing the gravitational effect of a refence density model, is possible to get the so-called "gravity anomalies", reflecting the presence of lateral density variations.

The subsurface density distribution can be modelled from the observed gravity anomalies by solving a non-linear inverse problem. Different geological and geophysical constrains must be used to reduce the range of possible mathematically coherent solutions. Only some models are geological meaningful.

The model can be limited to the upper crust (shallow and local density variations) or including the entire lithosphere (deep regional density variations) according to the geographical extension of the study area.

In regional studies, density is the key parameter controlling the mechanical behaviour of the lithosphere and can be used to understand the geological evolution in terms of isostatic adjustments and deformations induced by crustal loading.

The new dataset will be used to do a 3D gravity inversion and thermo-mechanical modelling 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 land 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 th 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 modelling will provide a detailed picture of the density structure of the lithosphere.
3. The density distribution in the lithosphere helps understand the vertical and horizontal movement/adjustment of the lithosphere (isostasy). 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. 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.

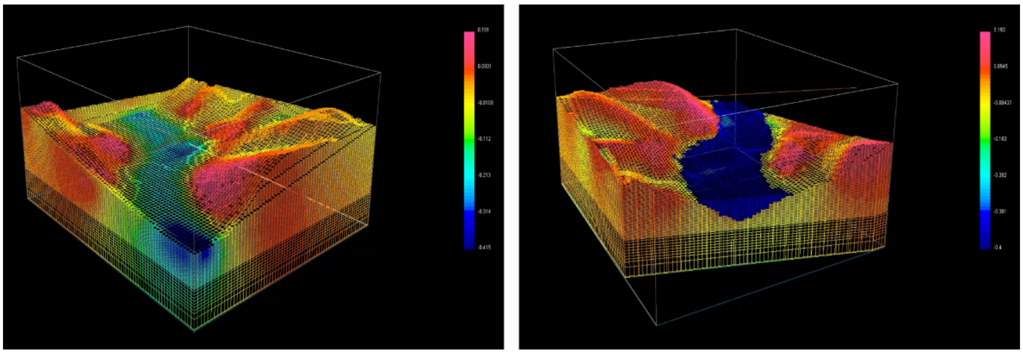

Fig.1 - Example of two possible density models obtained from the inversion gravity data of Lienz basin in the Austrian Alps (data provided by the Leibniz Institute of Applied Geophysics, Hannover). On the left the model obtained by solving the inverse problem without considering geometrical boundaries and on the right the same model constraining the geometry of the basin (blue body). Both models has been produced using the Grav3d software library.

Acknowledgement

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