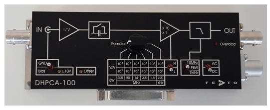
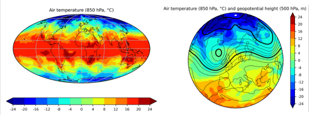
DEPARTMENT OF PHYSICS AND ASTRONOMY "AUGUSTO RIGHI"



ADVANCED SENSING LABORATORY



HIGH PERFORMANCE COMPUTING CLUSTER

ALMA MATER STUDIORUM UNIVERSITÀ DI BOLOGNA

OPH NEWSLETTER

FOCUS: Multiscale numerical modelling of the atmosphere

The Open Physics Hub (OPH) hosts a suite of numerical models to simulate **atmospheric and climatic processes** ranging from the urban scale to the global scale. These include general circulation models, mesoscale atmospheric models, radiative transfer models, dispersion models and computational fluid dynamics (CFD); a detailed description can be found at the following web page: https://physics-astronomy.unibo.it/en/research/projects-and-research-lines/research-lines/research-line-in-atmospheric-physics/modelling-tools

The infrastructure of the Open Physics Hub and the HPC cluster Matrix fostered the use and development of **massively parallel** and computationally demanding approaches. A noticeable example is the Open Integrated Forecasting System (OpenIFS), developed by the European Centre for Medium-Range Weather forecast (ECMWF) to promote research, teaching and training on numerical weather prediction. OpenIFS is a state-of-the-art **atmospheric general circulation model** (coupled to a land surface and to an ocean wave model) developed to deliver operational global high-resolution weather forecasts. The OpenIFS is currently in use in OPH following an agreement signed in 2021 between the Department of Physics and Astronomy "Augusto Righi" and the ECWMF and can support research on several topics such as analysis of the forecast and dynamics of high-impact events, development of model parameterizations and ensemble forecasting. An example of a retrospective forecast for an impactful event is shown in Figure 1.

The computational power of OPH is also employed in CFD applications for high-resolution numerical simulations of physical phenomena characterising the **lower atmosphere and urban scale**. The system supports OpenFOAM, an open-source tool-

Summary

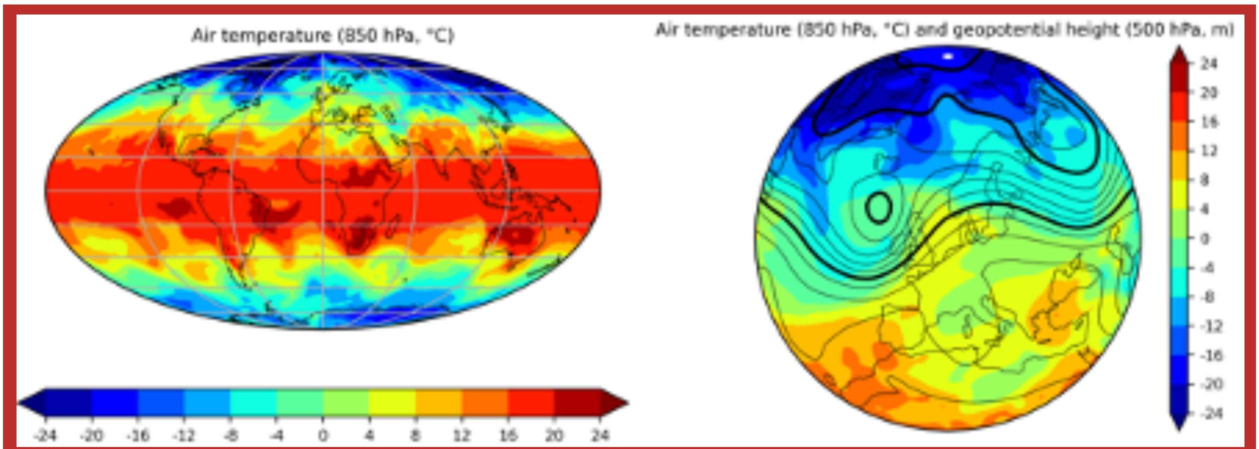


Figure 1. Example of a retrospective 96 h forecast reproduced with the Open-IFS in the Open Physics Hub for December 8th 2015 when an extra-tropical cyclone over the British Isles set the 24-hour rainfall record in the United Kingdom. The forecast has been reproduced with the latest version of Open-IFS (43r3) with a spectral truncation of T95. Left) Global field of air temperature at 850 hPa (°C). Right) Displayed fields are air temperature (shading, °C) and geopotential height (contours, m) on an isobaric surface of respectively 850 and 500 hPa.

box for numerical simulations that is increasingly popular and widely used. It allows various numerical approaches (e.g., Large-Eddy Simulation and Reynolds Averaged Navier-Stokes simulations) with accurate turbulence models. Original modules have been developed for the reproduction of phenomena such as natural convection, conjugate heat transfer, water evaporation and condensation, and thermal radiation. The extensive parallel computing resources make possible to realistically reproduce **complex thermo-fluid dynamical systems** and offering attractive educational activities that also include software development.

Finally, OPH is supporting the development of a **fully coupled climate model** of intermediate complexity (based on the existing Simplified Parameterizations Primitive Equations Dynamics, Molteni 2003, and the ocean model NEMO). This model features a three-dimensional representation of the atmospheric and oceanic dynamics along with parametrizations of other relevant Earth system processes (e.g., sea ice, convection, etc.). However, compared to the most recent comprehensive models, it achieves an optimal compromise between realism and simplicity of the parametrizations in order to make computations more affordable and fast. With such design, it can support innovative and explorative studies on crucial processes for Earth's climate evolution and variability but it can also be a valuable pedagogical tool to teach students how to run and use a climate model. Indeed, the aforementioned tools are currently used for practical hands-on sessions in many modules of the "Physics of the Earth System" master course.

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OPH: third year activity report

The third year of the OPH project has been a year devoted to the consolidation of the infrastructures and the activities started in the second year. The **High Performance Computing (HPC) Cluster** has been continuously running during the whole year. In two occasions, it was enlarged with new server blades and new storage capacity acquired on ERC and other funds. As a result, the current computation capability has roughly doubled with respect to the first installation. The **Advanced Sensing Lab** has provided the basis for on-the-edge research, even in the pandemic conditions. In particular, an experiment was performed at GSI (Darmstadt - GE) exploiting a ^{16}O beam, and the data was acquired with the help of OPH equipment. All these activities have led to **22 publications** on peer-reviewed journals, in collaboration with other UNIBO departments or other universities world-wide.

In addition to the base research, within OPH there is a consistent activity of **commissioned research**: several contracts with firms have been signed by OPH and DIFA researchers (13 at least clearly linked to OPH infrastructures and activities). Clearly, the availability of OPH helps DIFA's researchers preparing their competitive projects in search for fundings: we plan to use OPH as a leverage to further show capabilities and infrastructures to conduct top-of-the-class research projects. OPH has been mentioned in several **submitted projects** during 2021, and in **6 winning projects** (Horizon 2020 and MIUR) funded in the third year of OPH. Moreover, OPH infrastructures help young researchers and PhD students to make their challenging research projects possible, as reported regularly in our newsletter.

In addition to boosting research activities of the department and related research institutes, OPH has been involved in the **teaching improvements**. Many courses on computing, on simulations, on sensors and on electronics in our degrees have direct link to the OPH activities. In 2021, **14 master's and 11 bachelor's students** have prepared their thesis taking advantage of the equipment of the Advanced Sensing Lab as well as the HPC cluster.

Despite the pandemic, even in 2021 we held our **summer school** "International Summer School on Physical Sensing and Processing", https://www.unibo.it/en/teaching/summer-and-winter-schools/2021/physical-sensing-and-processing, in partnership with Universities around the world, research institutes and multinational firms (MacQuarie University, Stellenbosch University, MIT, Princeton University, Flinders University, Granada University, UCLA, CNR, CINECA, CBS Netherlands, INFN, Formica Blu). The event was held online-only and it attracted many Master and PhD students, mostly from Europe (see also OPH newsletter nr 4).

Among the activities performed within OPH, we had a structured **outreach program** connected to the PLS project (see details at pag. 4). With the help of the OPH funds and together with other funds, at DIFA we hired **2 post-docs** for two years: these constitutes the last hiring foreseen in 2018 at the time of the project writings, but they will not be the last one working on OPH research, for sure!

In summary, these activities represent part of the enormous potential of OPH. We expect that the best has still to come in the next years, when travels, researcher exchanges and meetings in person will return to be the main way to make advances in fundamental and applied research.

OPH 3RD YEAR IN NUMBERS

6 new funded projects (H2020 &MIUR)

13 third-party research contract

+137 % HPC computing power

2 post-doc contracts

22 publications

25 theses (bachelor, master and PhD)

1 summer school for master and PhD students

6 short courses for high school students

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Teaching and outreach

DIFA and OPH meet high school students and teachers

In the first months of 2022, the DIFA hosted virtually **160 high school students**, **40 in-service teachers**, and **10 teacher-students** to participate in **four laboratories** within the **PLS program** for university orientation and teacher training (www.pls.unibo.it/it/fisica). The activities represented a context to outreach the aims, the structure, and the research carried out in the OPH project. The courses, of 20 hours each, covered four outstanding themes of physics that are at the core of OPH as well:

- "*Electrons and photons from atoms to solids*" (Prof. Daniela Cavalcoli, Prof. Beatrice Fraboni, Prof. Federico Boscherini, Giovanni Armaroli, Ilaria Fratelli, Alberto Piccioni)
- "*Big data and networks between physics and biology*" (Prof. Daniel Remondini, Prof. Claudia Sala, Alessandra Merlotti, Francesco Durazzi),
- "*Simulations of complex systems*" (Prof. Olivia Levrini, Prof. Daniele Bonacorsi, Eleonora Barelli), and
- "*The second quantum revolution*" (Prof. Olivia Levrini, Prof. Elisa Ercolessi, Sara Satanassi, Paola Fantini).

In the courses, **several different activities** were organized for the high school students, including lectures, team works, virtual lab sessions, panels with experts, and collective discussions. The aim of the laboratories was not only to make participants develop technical skills and enrich their knowledge of the topics at stake. Dealing with **STEM issues**, at the intersection of Science, Technology, Engineering, and Mathematics, the students were guided to understand how nowadays the physicists **need to act in synergy with researchers in other fields** and with different stakeholders in order to respond in an interdisciplinary way to the current challenges of our society in rapid transformation.

The **PLS laboratories** were a precious opportunity of outreach to disseminate and raise awareness on the expertise in computation and simulation of the DIFA to societal stakeholders that do not strictly belong to the academia, like high school students and teachers. To their realization, it was fundamental the involvement of many "DIFA people" who presented first-hand their research on the topics. For example, in the laboratory on Simulations of complex systems, five Ph.D. students and **early career researchers** (Dr. Leonardo Aragão, Dr. Silvia Biondi, Matteo Billi, Francesco Durazzi, and Carlo Emilio Montanari) were involved as panelists in a round table to describe their research experience with simulations in different fields (epidemiology, nuclear physics, accelerator physics, climatology, astronomy).

The value of this activity was double. On one side, the young participants in the course had the chance to see how **interdisciplinary** the research in a physics department can be. On the other, the panelists themselves had the opportunity to **network** with each other and recognize similarities and peculiarities of their own investigations when confronting with the same family of computational tools.

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Teaching and outreach

The 4TH edition of THE DIFA International Summer School on Physical Sensing and Processing

A century after the great achievements of Quantum Mechanics, we are witnessing a Second Revolution. Our ability to manipulate single quantum objects and control quantum resources is at the heart of formidable advances that are expected to deeply influence and change our future. The IV Edition of the OPH Summer School on Physical Sensing and Processing will be dedicated to: Quantum Sensing, Information processing and Computing: shaping the future with the second quantum revolution.

It will be held in presence at the Department of Physics and Astronomy from 14^{th} to 20^{th} of July, 2022 and is meant to introduce Master and PhD Students to the fundamentals of Quantum Sciences and Technologies from both a theoretical and an experimental perspective, with an interdisciplinary approach.

Main lectures will cover the four topics of:
- Quantum Information
- Simulation
- Computation
- Sensing

They will be complemented by seminars on specific research topics that will address applications in various fields of physics and other scientific areas as well as presentations of public and private research centers working in the field of quantum sciences and technologies. Collaborative activities will be planned to support creative thinking and the development of transversal, soft and social skills.

Speakers will include professors and researchers from University of Bologna and the partner institutions of Brown University, MacQuarie University and Stellenbosch University, together with researchers from other public institutions and private companies.

Details can be found at the dedicated webpage.

(From: Quantum Manifesto, 2016)

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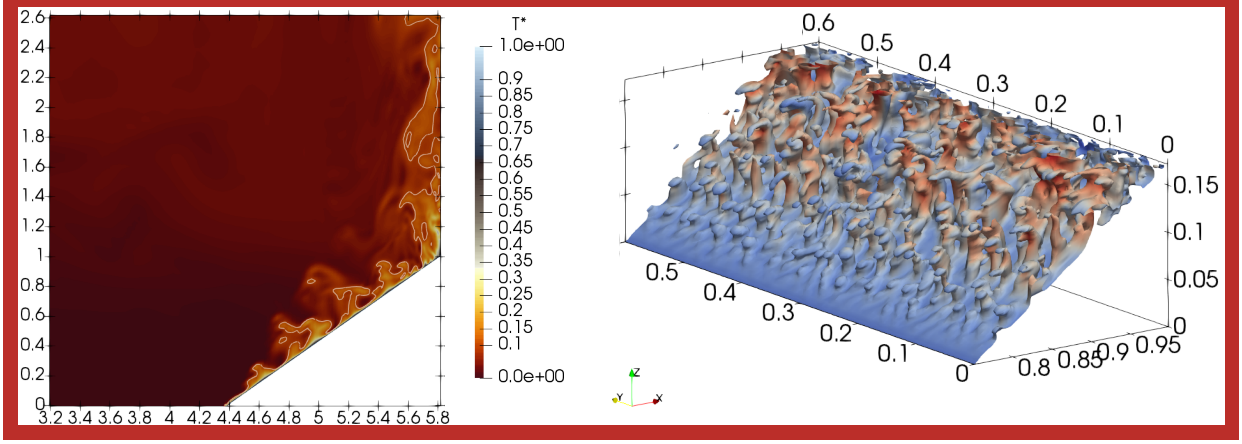
Publications related to OPH

TURBULENT STRUCTURES OF ANABATIC WINDS IN SLOPPING TERRAINS

Anabatic flows are thermally driven winds arising in sloping terrains, which significantly affect the dynamics and the exchange of mass and momentum in the low atmosphere. Because of the strong coupling between buoyancy and inertial forces, experimental and numerical study of such flows are particularly challenging and very few studies in literature have tackled this topic. The research group in Atmospheric Physics of the DIFA, led by prof. Di Sabatino, starts to investigate this phenomenon by high-resolved numerical simulation utilizing cutting edge Computational Fluid Dynamics techniques. Simplified geometry [1] and laboratory apparatus [2] have been numerically reproduced. The analysis of instantaneous fields reveals the presence of thermal plumes (see Figure 1), which are stable turbulent structures enhancing vertical transport and mixing of momentum and temperature [3]. Such structures are generated by thermal instabilities in the conductive layer that trigger the rise of the plumes above them. To the best of the authors' knowledge, such turbulent structures have not been described before.

Instantaneous visualization of turbulent thermal plumes arising at the slope surface.



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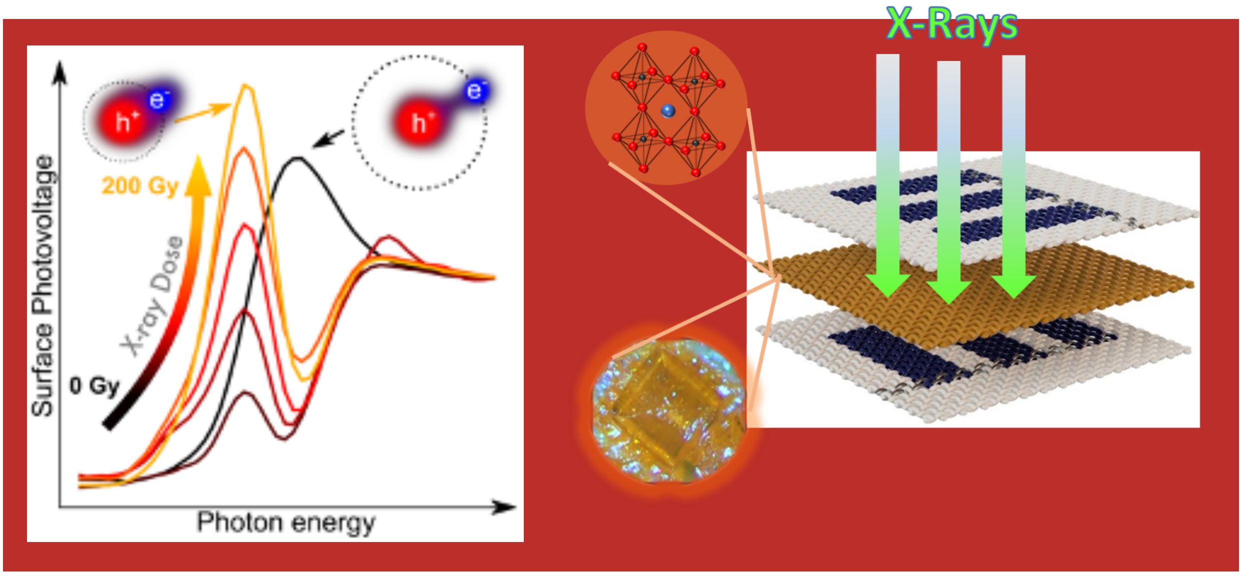
Publications related to OPH

EFFECT OF X-RAY IRRADIATION ON THE PHOTO-PHYSICAL PROPERTIES OF PEROVSKITE SINGLE CRYSTALS

Hybrid halide perovskite have recently attracted an increasing interest for the next generation of low cost and widespread optoelectronic devices, like LEDs, photodetectors, and photovoltaic cells. In this framework, lead-halide perovskite single crystals demonstrate to be excellent active layers for direct X-ray and gamma-ray detectors with outstanding sensitivity and low limit of detection [1]. The researchers at DIFA, led by Prof. D. Cavalcoli, carried out a study about the effects of prolonged exposure to X-ray irradiation on the opto-electronic properties of this material in order to test its radiation hardness [2]. Irradiation facilities (tungsten target X-ray tube) and material characterization techniques (surface photovoltage spectroscopy and photoluminescence spectroscopy) available at OPH Advance Sensing Lab have been used to probe photo-physical properties. Strong X-ray induced change in the excitonic properties of the material have been observed, even if their effect is not permanent as they a recovery effect occurs in the timescale of days.
The versatility of solution-processed perovskites allows the development of sensors with a new conceptual design. A fascinating example is described in the work presented by the team of Prof. B. Fraboni: a fully textile direct X-ray detectors, where the photoactive layer is constituted by a silk-satin fabric functionalized with methylammonium lead bromide perovskite crystals embedded in the textile [3].



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Contacts

OPH Spokesperson: Andrea Cimatti
OPH Coordinator: Mauro Villa
OPH Contact Point: Claudia Sciommeri
OPH Computing Facilities: Marco Baldi
OPH Advanced Sensing Lab: Cristian Massimi
OPH Newsletter: Filippo Zaniboni, Cristian Massimi

Useful links

OPH website
Department of Physics and Astronomy "A. Righi"
INFN
CNAF
OPH Computing Cluster user guide
International Summer School on Physical Sensing and Processing
Astronomy Public Conferences

OPH Newsletter: previous numbers

#1 OPH_Newsletter_01_May 2020
#2 OPH_Newsletter_02_Februay 2021
#3 OPH_Newsletter_03_May 2021
#4 OPH_Newsletter_04_November 2021

Edited by
Filippo Zaniboni
Cristian Massimi

Contributions
Giovanni Armaroli
Francesco Barbano
Eleonora Barelli
Andrea Ciavatti
Carlo Cintolesi
Silvana Di Sabatino
Elisa Ercolessi
Daniel Remondini
Paolo Ruggieri
Mauro Villa
Isabella Zironi

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