

New Trends in Physics Education Research

Salvatore Magazù

Editor

NOVA

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EDUCATION IN A COMPETITIVE AND GLOBALIZING WORLD

NEW TRENDS IN PHYSICS EDUCATION RESEARCH

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**NEW TRENDS IN PHYSICS
EDUCATION RESEARCH**

**SALVATORE MAGAZÙ
EDITOR**



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Additional color graphics may be available in the e-book version of this book.

Library of Congress Cataloging-in-Publication Data

ISBN: ; 9: /3/75835/: ; 6/: "gDqqm"

Published by Nova Science Publishers, Inc. † New York

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PREFACE

The main aims of the Special Issue titled *New Trends in Physics Education Research*, is to deal with new trends in teaching and learning processes in Physics, to highlight new Mathematics contents for Physics courses, to put into evidence the key role played by laboratory activities in Physics training courses and to stress the importance of communication and dissemination of scientific culture.

Physics teaching involves several fields and different disciplines, such as Mathematics and laboratory activities. In particular, Mathematics and Physics are two distinguished disciplines that can generate difficulties to students in learning some concepts. It often happens that the same arguments are explained in different ways, without clarifying that there is a close correlation between the two disciplines. In this framework, an integrated theoretical and experimental approach can improve the knowledge of some subjects of Physics and Mathematics; furthermore, it is also useful to employ a joint approach with laboratory activities, so enriching topics of meaning. Mathematics provides the adapt tools for Physics and also is able to drive physical intuition; on the other hand, Physics and its laboratory activities provide a simple access to Mathematical topics of complex comprehension. The issue is addressed to academic and school teachers as well as to researchers in the field of Physics education.

The issue is divided in 13 chapters.

In chapter one, the author observes that several poets in the past believed, after the cultural revolution in the seventeenth century, that science was killing the beauty of art and poetry, although opinions were generally discordant in intellectual classes. For that reason, it was long believed that imagination has been believed as opposite to scientific method. The author explains that this point of view has been generally abandoned with time, and now the role of imagination in science is well recognized as an essential ingredient. Recent research activity is reported to show some examples of how imagination can help in setting up smart procedures to prepare novel materials in modern science. Some directions are also suggested.

In chapter two, the authors put into evidence that questionnaires are widely used instruments to assess conceptual learning in Physics as well as in Mathematics. They discuss two Cluster Analysis methods that are able to identify groups of students that are homogeneous with respect to the ways students use to answer a questionnaire.

In chapter three, the authors deal with strategies and approaches on how to develop a Physics curriculum for undergraduate students that includes computing as a central element. The chapter begins with a definition of computing and pertinent learning outcomes and assessment studies and programs; then it ends with a discussion on how to implement computing in various Physics courses. Experiences from Michigan State University in the USA and the University of Oslo in Norway are reported.

In chapter four, the authors perform an analysis of the relationship between Mathematics and Physics. They deal with the kind of connections and integrations which are needed to design a class initiative which is oriented towards the teaching of skills. In particular, the authors propose a laboratory for higher secondary schools on Bréguet's spiral. The proposed laboratory uses computers with the aid of the dynamic geometry GeoGebra software, which allows to produce a simulation of reality with the help of the geometrical model.

In chapter five, the author deals with the recent discoveries in nanoscience and nanotechnology highlighting the enhanced powerful methods of supramolecular approaches, which are based on the complex combinations of different forces which act at the molecular and supramolecular levels. A review of the evolution of the concept of force in connection with recent discoveries in the field of nanotechnology, with the special focus on the development of modern approaches in academic physics programs, is presented.

In chapter six, the authors put into evidence the advantages to adopt an integrated mathematical and physical approach in teaching Fourier and Wavelet analysis. On that score, they report the results of an experiment on a variable length conic pendulum, putting into evidence how the Wavelet Transform, differently from the Fourier Transform, easily allows to get information on the time evolution of the registered signal frequency content.

In chapter seven, the authors deal with a subject of great importance in advanced Thermodynamics curricula: the adiabatic piston problem. By using an appropriate kinetic model they determine the final state of the system. It is shown how it is possible to evaluate the phase relations between temperature and piston displacement by applying the Wavelet Cross Correlation approach. Furthermore, relevant physical parameters are analysed by applying the Fourier transform approach.

In chapter eight, the authors show how acoustic levitation furnishes an effective and straightforward technique to explain acoustic standing waves. Furthermore, a study of the damped oscillations of acoustically levitated spheres is presented. For the interpretation

of the data two mechanical mathematical models, which make reference to harmonic and damped oscillations, are introduced.

In chapter nine, the authors deals with meteorological maps. In particular, the authors explain how a meteorological map is built, what exactly mean the symbols represented on the maps and how they are produced. Starting from a short history of meteorology during last 300 years, they arrive to describe the modern methodologies to produce and plot synoptic charts by means of computer and specific software.

In chapter ten, the authors report a case study addressed to scientific curricula graduate students, concerning the application of Fourier Transform (FT) and Wavelet Transform (WT) on climate data and on their connections with Milankovitch's cycles. From the FT and WT analyses, it emerges that, in the last 500000 years, the presence of glacial maxima with time intervals of around 100000 years, connected with the variation of the eccentricity of the Earth's orbit, is revealed. Moreover, between 1.8 and 1.3 million years ago, glacial maxima repeat about every 41.000 years, in agreement with the cycle of variation of the Earth's axis inclination

In chapter eleven, the authors propose a conceptual map for a multidisciplinary approach of the post-graduate programs in soft condensed matter physics, one of the most important field in modern science and technology. Highlighting the synergistic relation and the conceptual interconnection between different parts of the field, may stimulate the exploration of new solutions for a multi- and inter-disciplinary integration of knowledge and skills.

In chapter twelve, the authors represent the expression for the “generalized” Wien’s displacement law of thermal radiation of a real-body by means of a limited number of frequency moments. In particular, they distinguish that in the case of blackbody radiation this expression is transformed into the well-known Wien displacement law. They study the temperature dependence of the “generalized” Wien displacement law for several metals such as carbides, luminous-flames, and the quasi-periodic micro-structured silicon coated with 100 nm thick Au film, showing that in the case of high temperatures the Wien’s displacement law decreases linearly with increasing the temperature.

In chapter thirteen, the authors deal with the study of the structural and dynamic processes occurring in biological membranes which represents a central topic in many aspects on science. Those processes involve collective behaviour of a great number of interacting molecules, while the understanding of structure-function relationship require the simultaneous calculation (and simulation) of a large number of parameters. Self-assembly processes in biomembranes represents the cornerstone of functioning of biological systems, resulting in the synthesis of complex macromolecular assemblies containing protein, nucleic acid, lipid and carbohydrate components. In this chapter, we illustrate some of the main approaches and techniques applied for the study of biological membranes and the multitude of processes occurring simultaneously in a wide range of the space-time domain. The future challenge in this research field must provide the

integration of the different research/teaching models into a common background based on multi- and interdisciplinary approaches that combine the expertise coming from the different disciplines.

ACKNOWLEDGMENTS

As Guest Editor, I would like to express my appreciation and thanks to all the contributing authors and to reviewers who have provided constructive reports in a timely fashion. I am confident that the final outcome reports a balanced representation of the field and points out the perspectives for future developments.

Finally, I would greatly appreciate to thank the Nova Publisher Editors and the Technical Staff for the kind courtesy and the precious support in the publication of this Special Issue.

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Chapter 1

MANAGING COMPLEXITY IN MATERIAL SCIENCE: THE ROLE OF IMAGINATION

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ABSTRACT

Several poets in the past believed, after the Cultural Revolution in the seventeenth century, that science was killing the beauty of art and poetry, although opinions were generally discordant in intellectual classes. For this reason, imagination has been believed to be as opposite to scientific method. This point of view, luckily, has been generally abandoned with time, and now the role of imagination in science is well recognized as an essential ingredient. Recent research activity is reported to show some examples of how imagination can help in setting up smart procedures to prepare novel materials in modern science. Some directions are also suggested.

Keywords: imagination, material science, soft-matter, complexity, emerging properties, creativity, nanotechnology

THE PROBLEMATICS

This chapter was inspired by the article "The role of imagination in science: van't Hoff's inaugural address" dated 1960 [1]. I will therefore present my ideas on the role of imagination in material science, a role which may even approach that of *creativity* or even *fantasy*. I can imagine that for most readers it may be embarrassing to deal with the creative faculties of mind in scientific fields. Indeed, it is known that any scientific model

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must be subjected to the validation operated by well-defined experiments. Moreover, the unavoidable requirement is that such experiments must be repeatable, meaning that the results, within a certain and accepted uncertainty, must be always the same. In this scenario, science may look as a rigid framework where all the relationships between causes and effects or, in words better suited for material science, between molecular constituents and the overall system properties are dictated by mathematical rules and physical laws. This common belief would be the result of the Cultural Revolution occurred in the seventeenth century. In that period, the role of imagination has been weakened even in arts. From that age, uncontested progresses in the field of physics occurred especially in the last century and, later, in chemistry and in material science. This allowed an unprecedentedly detailed vision of the reality around us giving strength to rationalism and reinforcing the scientific vision of defined relationships between theory, models and experiments. This strong and powerful approach actually delivered efficient tools to manipulate matter: there are tangible proofs (possibility of human beings cloning, electronic devices which have revolutionized our life etc.) that the rules of life seem well-known and that the knowledge in physics at the base of technological progress looks well set up. In this scenario, the idea that there is no room for imagination and creativity seems to be justified, but in reality it comes from preliminary and superficial considerations: imagination plays, instead, an important role in the capacity to carry out scientific research both in the interpretation of natural phenomena and, with specific reference to material science, in the utilization of the knowledge to invent new materials and devices. In material science, in fact, the smallest building blocks must be stable components of matter i.e., atoms and molecules which are organized to form bigger structures. Atoms are assembled to form molecules, molecules can be assembled to form supramolecular aggregates, these are organized to form living cells and so on, in escalation which can have a high number of levels. In a complex assembly the property does not come from the properties of the building blocks because new and unexpected emerging properties can arise when passing from a level to another. Imagination is of pivotal importance in exploiting the possibilities of having emerging properties in complex systems.

Far from being a review on the role of imagination in material science, the aim of this contribution will be just to give some comments hoping they may be useful for the curious reader to find connections between the fascinating world of imagination-driven attitude and the rigorous world of scientific progress in material science.

THE LONG DEBATE ON IMAGINATION

This topic is obviously not new. The first comments in this sense can be traced back to around 1600, i.e., when the Scientific Revolution took place. Copernicus' "De

revolutionibus orbium coelestium" is, in fact, dated 1543 and "*Philosophiae Naturalis Principia Mathematica*" by Isaac Newton (1642-1727) was published in 1687. Reporting comments from the past is useful to depict the cultural background where the role of imagination and creativity has grown up. The mathematical/analytical approach of science was despised by a lot of poets and writers: William Blake (1757-1827), in his *Laocoön* clearly writes that the art is the tree of life, whereas the science is the tree of death; Heinrich von Kleist (1777-1811) argued that Isaac Newton would have seen, in the fascinating features of a beautiful woman, only curved lines and in her heart just its volumetric capacity. The following argument by David Herbert Richard Lawrence (1885-1930) is particularly explanatory:

‘Knowledge’ has killed the sun, making it a ball of gas, with spots; ‘knowledge’ has killed the moon, it is a dead little earth pitted with extinct craters as with smallpox; the machine has killed the earth for us, making it a surface, more or less bumpy, that you travel over [2].

On the other side, John Tyndall's belief is that such common sense is just the consequence of lack in knowledge [3]. Tyndall was born in 1820 and worked as a surveyor and as engineer: for this reason he got his degree in Physics only in 1850. However, after that, his contribution to science popularization is with no doubt inestimable. It is not a case that Tyndall became friend of Michael Faraday (1791-1867), who is generally held to be one of the greatest experimental philosophers of all times. Faraday, on his side, had to overcome even more difficulties before fully dedicating himself to science: after an elementary education, consisting, in his own words, of ‘little more than the rudiments of reading, writing and arithmetic’, Faraday left school at the age of thirteen [4]. However, his imaginative view of the concepts, which he has learnt successively, helped him to develop works “with numerous illustrations” [5]. Both scientists shared the opinion that imagination is an essential element in science.

This debate has been hot also in other fields: after Isaac Newton explained the origin of the colors of the rainbow in terms of dispersion and reflection of light in the minuscule water droplets suspended in the air [6], the poet James Thomson (1700-1748) wrote [7] “How just, how beauteous the refractive law” thus emphasizing the role of scientific knowledge in enhancing the beauty of the rainbow. John Keats (1795-1821), instead, believed that Isaac Newton destroyed the poetry of the rainbow by “reducing it to the prismatic colors” [8]. This accusation inspired, in turn, Richard Dawkins' book, dated 1998, entitled “Unweaving the Rainbow” (subtitled “Science, Delusion and the Appetite for Wonder”) where the Author showed that science does not destroy, but rather discovers poetry in the patterns of nature: “Keats could hardly have been more wrong,” it seems he has said.

Mark Akenside (1721–1770, poet and physician) had the same opinion:

Man loves knowledge, and the beams of truth
More welcome touch his understanding's eye
Than all the blandishments of sound his ear,
Than all of taste his tongue [9].

An opinion which was still present in other popular people like, just as mere examples, the poet Hugh MacDiarmid (1892-1978) and the scientist Richard Feynman [10] (1918-1988).

As it can be seen, opinions have been diverse, but it is important to notice that a conspicuous number of people supported the progress in science not as putting poetry, human feelings and imagination at risk, but rather enhancing them. If we support this point of view about the effect of scientific progress in imagination, we should also consider, on the other hand, the vice versa, i.e., the effect of imagination in science. In this regard, some examples on how imagination has helped scientists in their work can be useful. Let me begin with the peculiar case of the scientist Jacobus Henricus van't Hoff (1852-1911), the scientist who inspired this contribution. He was a Nobel Prize in 1901 for his studies in the physical chemistry of solutions and osmotic pressure. Well known is, in fact, the so-called "van't Hoff coefficient" (usually indicated by the letter i) indicating the effect of electrolyte dissociation in colligative properties of solutions. However, few people probably know that his first scientific intuition does not regard the chemistry of solution but, rather, the stereochemistry. During his PhD studentship, in fact, he was particularly involved in the relationship between the chemical constitution of organic compounds and the possibility for some of them to have specific optical rotation or activity. He reputed that the 2D representation of chemical formulae as drawn on a paper sheet, was absolutely unsatisfactory, so, considering the possibility for carbon atom to form four bonds, he first had the intuition that the tetrahedral distribution of chemical bonds around the carbon atom could justify a lot of phenomena still waiting for clarifications, including the existence of isomers. Actually, after Louis Pasteur's (1822-1895) observation that tartaric acid recovered from recipients for wine production were able to rotate the plane of polarized light, it can be said that stereochemistry was born thanks to van't Hoff hypothesis (to be honest also Joseph Achille Le Bel (1847-1930) had the same idea more or less at the same time). The scientist of course published his conjectures, but he was quite unlucky: the scientific community opinion was initially against him and the idea of atoms spatially distributed according to specific and atom-dependent local geometry was accepted only after the publication in 1875 of the *Chimie dans l'espace* (Rotterdam, 1875). After this experience he held a lesson "the power of imagination in science" where he explained the important role of imagination in science. Science, in fact, has an aim, i.e., to find the relationship between causes and effects and, in this search, imagination cannot but having a pivotal role. In deeper details, the process has two steps: i) the observation of a phenomenon and ii) the search for cause-effect

relationship. In the first step imagination is essential not only in the choice of the exact moment (and nature) of observation, but also in the choice and eventually the change of the experimental conditions of the observation in order to have a more significant inspection. But imagination is essential also, and probably more evidently, in the second step, and specifically in the search for the link between causes and effects, exploring the most opportune, even sometimes indirect, pathways; imagination is essential in developing hypothesis bridging the previous knowledge with the new and still to rationalize phenomena. This process is schematically depicted in Figure 1.

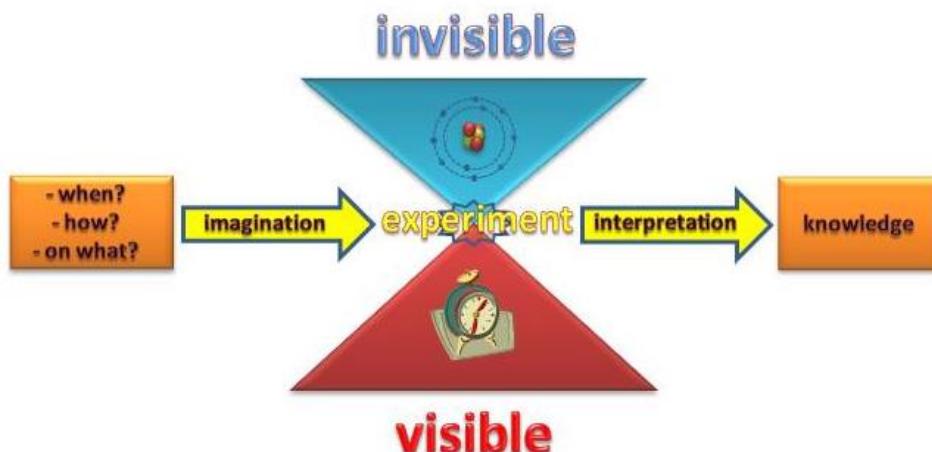


Figure 1. Re-adaptation of van't Hoff belief on the role of imagination in science.

Specifically in material science, discovering the particular arrangement of a number of atoms/molecules of the order of Avogadro Number ($\sim 10^{23}$) to vive the specific observed property, needs surely some imagination.

In few words, imagination is the capability to visualize an object with all its properties in such a way that it can be represented with the same precision as in a direct observation: in the specific case, van't Hoff had imagined the tetrahedral local geometry around carbon and this has been later experimentally confirmed by X-ray diffraction.

In van't Hoff belief, the job of a scientist must proceed through observation and imagination if important results are desired. We all know that, sometimes, important results are obtained through a constant work to realize some idea which was initially only in the researcher's mind as a result of mere imagination.

Another representative example can the teaching of Friedrich August Kekulé (1829-1896): he hold a lecture in 1890 in occasion of the *Benzolfest* organized in the Berlin City Hall to explain how carbon atoms are able to bind each other to form complex structures (chain-like or cyclic as in aromatic compounds). He reported quite mythical episodes as at the origin of his theories: he declared to have hypothesized the cyclic structure of benzene after a dream populated by snakes, one of which had bitten its own tail to form a

ring. It is not clear if this really happened but what is certain is that Kekulé used this story to strongly invite scientists in having imagination and in following it to develop hypothesis. Of course their verification through the light of the scientific approach and through rigorous tests still remains a necessary step.

The same approach seems to be characteristic of Dmitrij Mendeleev (1834-0907), the father of the periodic table, who deliberately mixed his discovery of the periodic table with myths and legends. It is told that in date 16 February 1869, Mendeleev had a dream, in which the chemical elements would have appeared to him as ordered in his periodic table. After waking up, Mendeleev would have then worked hard to write down the details of his dream. As the reader can see, there is again the use of dreams to show how a discovery has been made. Other legends are actually present but their narration is not the scope of this contribution. Rather, what is important here is to show how scientists generally make use of fantasy to tell their stories. Coming back to the case of Mendeleev, in another legend he would had prepared a card for each of the known elements and then he started playing with them like in a patience with game cards, finding at the end the exact position for all of them. Beyond the tale, it is reasonable that the scientist has worked hard in finding the exact order of the known elements, like in a puzzle. So this story, rather than being considered a legend, should be seen as the "real" fact i.e., that the scientist has worked hard to solve the problem. Like in any complex problem to solve, with countless possible moves but with only one correct final configuration, imagination and intuition help, and probably Mendeleev in his story wanted to emphasize more the role of imagination/intuition rather than that of his undoubted efforts.

COMPLEXITY AND IMAGINATION IN MATERIAL SCIENCE

In material science the smallest building blocks are obviously atoms about which much is already discussed in the previous chapter. They need, in their first step, to be organized to form definite nanostructures. Such nanostructures can then arrange themselves to form the macroscopic material. In this self-assembly process, which starts from the atomic-lengthscale and ends up to the macro-lengthscale, there is a complex pattern. Indeed, at the nanoscale, below a substance-specific size threshold, the properties of many solids becomes strongly size-dependent due to quantum size effects and it cannot be neglected that a considerable fraction of surface atoms are in contact with the surrounding medium: surface adsorption of suitable molecules besides stabilizing the nanoparticles, offer a chemical modification (functionalization) which is the first step for their piloted assembly. As a consequence of all these considerations, the preparation of a material with desired characteristics is based on a simultaneous exploitation of the following strategies:

- 1) the synthesis of new molecules (synthetic chemistry);
- 2) the blending of already known materials;
- 3) the reduction of the dimensionality of already known materials to the state of nanoparticles, nanowires, nanoplates which simultaneously takes into account the need in miniaturization.

These strategies are depicted in Figure 2, left part of the tree, grouped into the “known strategies.” At the base of the scheme the starting point is indicated.

All these aspects can constitute different topics in physics education, rendering the approach for the study/preparation of modern materials particularly dispersive and disorganized. This would be detriment for student education in academic courses. A winning approach can be the rationalization in terms of complex behavior of matter and materials.

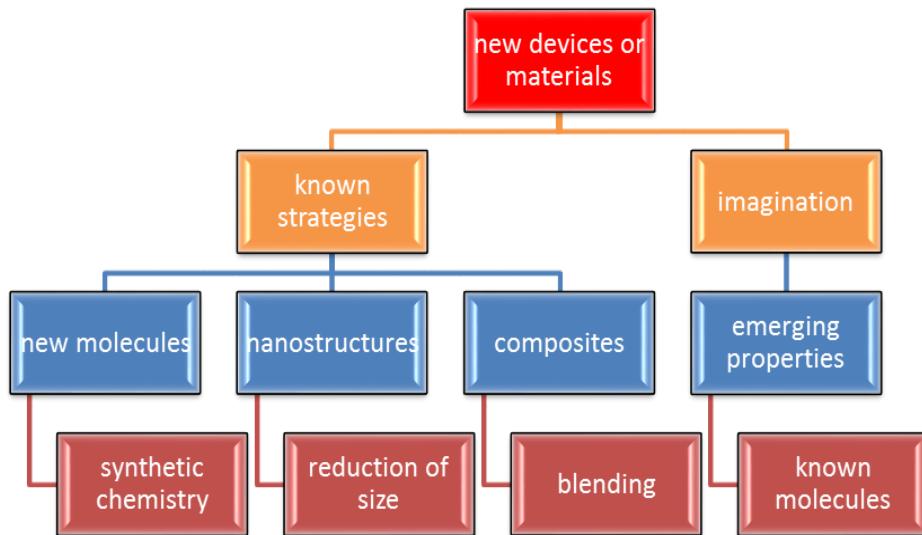


Figure 2. Scheme of the strategies used to build up new devices or materials in materials science.

Complexity, in fact, deals with the organization of units to form bigger entities which are ultimately constituted by the opportune arrangement of those sub-units. This is true in any kind: from chemistry to computer programming to sociology. Just to introduce the topic by an example, elementary particles are somehow assembled to form atoms (physics), atoms are assembled to form molecules (chemistry), molecules can be assembled to form living cell (biology), opportunely organized living cells can constitute tissues (physiology, medicine), and so on, organs, human beings, society... in a multi-step escalation which can have a big number of levels. This is schematically depicted in Figure 3 and, from another prospect, in Figure 4.

If a system was the bare collection of independent and non-interacting constituents, it would be just a “simple” assembly of its constituents: most of its characteristics could be predicted from the characteristics of its constituents. Instead, if the constituents are interacting, the complex assembly is not the mere collection of its building blocks and the overall properties cannot be obtained by simple extrapolation of the characteristics of their constituents: new and sometimes unexpected emerging properties can arise when passing from a level to another.

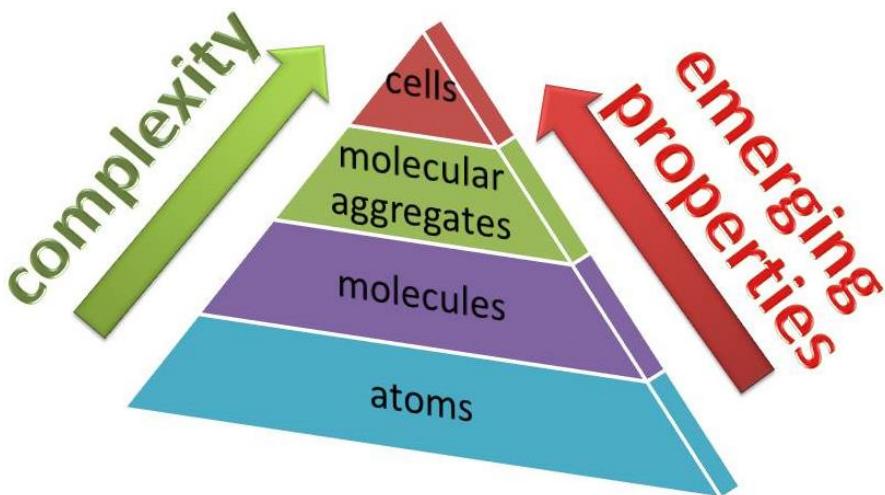


Figure 3. Increasing levels of complexity generate systems with emerging properties and novel functionalities. In the case of a cell, it is constituted by supra-molecular aggregates, which, in turn, are constituted by molecules and, at a lower level of complexity, by atoms.

Formally, a simple behavior can be envisaged when an overall system property (P_l , where the subscript refers to the level of complexity labelled "l") is the mere sum of the properties of all its i constituents obviously lying at a lower ($l-1$) level of complexity. (See eq. 1.)

$$\text{simple system: } P_l = \sum_i P_{l-1}(i) \quad (1)$$

$$\text{complex system: } P_l = \sum_i P_{l-1}(i) + f[1,2,3,\dots,n] \quad (2)$$

The mass for example, which is usually a simply additive property, has simple behavior. Instead, a complex behavior holds when there is a contribution specifically depending on the presence of all the building blocks in addition to the sum of the properties of all the constituents. Excess volume, for example, or any other excess property is explicitly defined in these terms. This further contribution, shown in eq. 2, originates just because of the simultaneous presence of the constituents. Excess mixing

volume between two liquids just originates because of the molecule-molecule interactions or even just because of different molecular sizes [11]. Therefore, another approach in modern materials science could be, in my opinion, the generation of new devices/materials exploiting the emerging properties shown by the assembly of already known constituents. This approach is parallel to the aforementioned one and is reported in Figure 2, right part of the tree. This approach, cannot but consider imagination and intuition as the driving force.

I strongly support the use of imagination in materials science. Not only imagination can give shortcuts in the understanding of the properties of novel materials in a well-organized experiment, as from the idea by van't Hoff, but, also, it can give intuition for the practical preparation of novel materials and of new devices. But imagination usually needs some episode as a starting point: for example, the exploitation of some emerging properties (high proton conductivity exceeding 10^{-3} S cm $^{-1}$ at high temperatures - above 100°C) by simple mix of already known materials for technological application was already observed by J.D. Kim et al. in 2005 who mixed benzimidazole and monododecyl phosphate acid [12]. This observation was explained in terms of two-dimensional proton-conducting pathways within the polar domains of highly ordered lamellar structures [13]. The details on the origin of these effects were better pointed in 2010 when we noticed that by mixing two opportunely chosen liquids a noticeable increase in proton conductivity could be obtained [14, 15]. In this framework, driven by our belief in complex behavior importance, we imagined this peculiar effect as the synergistic result of two effects: the H-bond formation and the intermolecular local self-assembly. In few words, the capability possessed by some surfactant molecules to form H bonds gives availability of "mobile" protons, and the consequent intermolecular self-assembly can constitute preferential pathways for their transport. Although this hypothesis drove us to prepare afterward systems with enhanced proton conductivity at low cost and by simple procedure [16], the idea was probably considered quite visionary, at least considering the reduced number of citations/repercussions in the literature in those years. Furthermore, we imagined that the coexistence of polar and apolar domains in the fluids could resemble the picture of self-assembly in ionic liquids [17]: instead of a spatial segregation of positive and negative charges [18] there is a segregation of polar and apolar nano-domains. Fortunately, our hypothesis turned out to be correct and the exploitation of this effect allowed us to get, by simply mixing two opportunely chosen surfactant liquids, anomalous 1D diffusion [19], exotic solubilizing properties towards inorganic salts [20, 21, 22], anti-Arrhenian behavior of proton conductivity [23] and even smart materials fully responsive to an external stimulus (magnetic field) [24]. As it can be seen, here imagination and the constant work inspired by the molecular picture we had imagined have allowed us to prepare various systems obtaining several novel properties.

The arising of emerging properties in complex systems opens the door to the soft matter field, which is one of the most important branches in modern material science.

Here, the same approach can be used: imagining the possibility to prepare soft matter-based materials not just by the opportune dispersion of nanoparticle in suitable matrixes, but also by giving the "soft" property to the particle themselves and observing how these properties can be amplified when such particles are organized.

One of the main characteristics of the self-assembly processes in soft nanomaterials is the weakness of the involved forces (so called "*soft interactions*" of the order of few kJ mol⁻¹) together with the involvement of a multiplicity of interaction sites [25, 26, 27, 28, 29]. The localization within the framework of complex systems can be individuated in Figure 4, which schematically represents the typical strengths and types of the interactions involved at the different levels of complexity. In the framework of soft matter, the weakness of the forces, jointly to the high number of interactions, require a substantial change in how these new topics must be addressed with respect to the traditional Newtonian framework. Despite the weakness of the interactions involved, the relevant number of these forces produces, indeed, an overall effect which is strong enough to hold together different molecular structures (building blocks) [30, 31, 32, 33, 34]. Detailed treatment of the main soft (non-covalent) forces acting in nanostructures self-assembly (such as the hydrogen bonding, hydrophobic effects, screened electrostatic interaction, steric repulsion and van der Waals forces) represents then a fundamental step for the understanding of the complex and cooperative behaviour in advanced functional materials [35, 36, 37, 38, 39]. This requests additional imaginative and creative efforts for the study of the corresponding multi-particles complex systems. The ability to draw hypotheses and design new experimental work within a research investigation represents a crucial step for the scientific work of a new generation of researchers. This requests a broader interdisciplinary scientific knowledge in connection with an integration of skills and a suitable dose of imagination and creativity. The role of soft interactions is particularly important in the constructions of nano-devices composed of heterogeneous components, as they govern the stability of component clusters, essential for the design of nanostructured materials and nanodevices [40, 41, 42, 43, 44]. The new technological paradigms that might be developed as a consequence of these fundamental studies promise new ways of thinking, where imagination and creativity can drive the choice of suitable models that help old problems to find the best approximate solution. Soft interactions, in fact, enhance the complexity and increase the ways in which multicomponent systems can interact, but also enlarge the range of the structural morphologies which are generated in the nano-structured materials involving these interactions, like liquids, suspensions, colloidal aggregates, biological systems [45, 46, 47, 48, 49]. In this respect, not only imagination, but also creativity, can help in modeling the complex many-body interactions, as well as the representation of the generated structured assemblies [50, 51, 52, 53].

Finally, few words cannot but being dedicated to nanotechnology (about which the possibility of building nanodevices has already been cited) since it is the current

predominant field in material science. Nanotechnology can be defined as the controlled manipulation of matter in space, time and chemical composition at the nanometer scale. Many different aspects are included: a work in the late '90s [54] already showed the results of a survey where various (twenty-two) experts working in different research areas were asked to indicate what they saw as nanotechnology. It turned out that nano- and quantum electronics, nanostructured materials and scanning probe microscopy were the most cited fields, being quoted by more than 17 researchers. Molecular materials for electronics and molecular nanotechnology were also considered as part of nanotechnology for 16 of the 22 experts. However, also computer modelling, cluster and mesoscopic science as well as technology and supramolecular chemistry were taken into account. As it can be seen there was no 100% consensus and many different fields need to be considered as part of nanotechnology. Moreover, due to the big differences among all the aforementioned disciplines, it is better to think of nanotechnology not as a unique field but just as a complex structure of interconnected research areas. It follows that co-operation among researchers in different disciplines is pivotal for the progress of nanotechnology deserving to be reinforced as much as possible. Consequently, it turns out that working interdisciplinarily needs imagination.

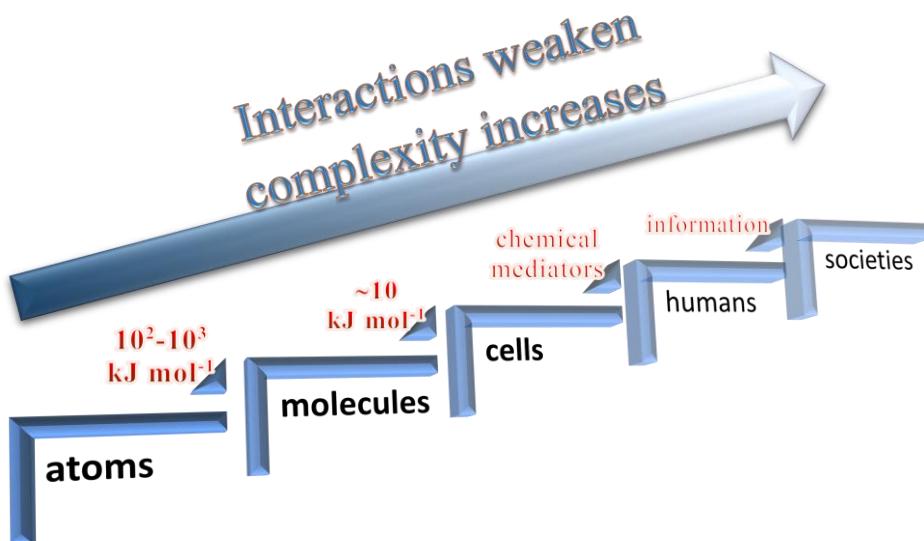


Figure 4. Schematic representation of the typical strengths and types of the interactions involved at the different levels of complexity.

In this ambit, in a scenario where nanostructure preparation were usually carried out either by bottom-up or by top-down methods, we went beyond by imagining an approach which could merge the merits of both: an hybrid approach which would simultaneously exploit the self-assembly of chemical species (bottom-up) and their formation from bulk precursors by physical methods (top-down) [55]. This imaginative attempt was successful

and simple, so laser ablation of target in liquid microemulsions, for example, are now well set-up methods [56, 57, 58] with the specific advantage to overcome some problems deriving by the mere utilization of chemical methods for preparing complex multi-element structures [59]. Of course, many other examples can be made, but a complete review of the activity in this sense would go beyond the scope of this contribution.

CONCLUSION

In conclusion, I believe that imagination plays an important role in the work of a researcher. The debate has been burning for centuries, but nowadays the idea that scientists must have an imaginative attitude is quite shared. Nevertheless, this is clear only in restricted sections of population, unfortunately. Therefore, in my opinion, the crucial role of imagination in science, and especially in material science, needs to be stressed even from the educational and academic courses to avoid the common sense that science imposes rigid schemes. Rather, imagination can furnish unprecedented points of view about all what surrounds us. As it turns out from examples of modern activity, the approach for a research based on interdisciplinarity represents a modern trend [60]. In this sense, borrowing concepts from the physics of complex systems, I like to see imagination also as an emerging property arising in complex research groups made by researchers with different expertises [61, 62]. Imagination is strikingly stimulated by the exchange of ideas among people with different points of view. It is advisable a shift from research to education. Teaching programs should take into account for this. They must require a method for giving student the correct approach allowing them to clearly identify each skill within the complex organization of scientific research [63, 64]. The development of a conceptual map is then desirable. It is necessary to go out of the single-discipline curricula, which have been traditionally sustained in traditional education, to switch to multi- and inter-disciplinary integration of knowledge and skills. This is a must, since students at any level are required to have such kind of attitude for a state-of-the art research. Apart from single-teacher intervention, a cooperative strategy is advisable. Research is already on the right way, but education is late. *Ad-hoc* actions in academic courses could speed up the process with great benefit for future students.

ACKNOWLEDGMENTS

Unpublished and published works by Prof. Vincenzo Schettino (University of Florence, Italy) have been very useful. They served as inspiration and furnished, at the same time, many useful information.

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Chapter 2

AN UNSUPERVISED QUANTITATIVE METHOD TO ANALYSE STUDENTS' ANSWERING STRATEGIES TO A QUESTIONNAIRE

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ABSTRACT

Questionnaires are perhaps the most widely used instruments to assess conceptual learning in physics as well as in mathematics. In the field of physics and mathematics education research it is surely interesting to be able to use a questionnaire as a “diagnostic instrument,” i.e., to know details about relationships among student answers to the different questions. In recent years several research works focused on this goal by using different quantitative methodologies, like Factor, Model and Cluster Analyses. However, very few research works deepened the theoretical aspects of the Cluster Analysis. In this contribution, we discuss two Cluster Analysis methods with respect to this issue. By means of an example of application on real data, groups of students homogeneous with respect to the ways students answer a questionnaire are identified. Each of these groups is identified without any prior knowledge of what form those groups would take (unsupervised classification) and can be characterised by means of the answering strategies the students deploy when facing the questionnaire. Each characterisation allowed us to infer the students’ lines of reasoning. Finally, we show to what extent the two clustering methods are coherent with each other.

Keywords: clustering, quantitative analysis, student reasoning lines

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INTRODUCTION

In the field of physics and mathematics education research, the answers given by students to a questionnaire are usually data from which it is possible to obtain information about student behaviour. Several quantitative research studies involving open- and closed-ended questionnaire analysis have provided instructors/teachers with tools to investigate students' conceptual knowledge of various fields of mathematics and physics (Bao and Redish 2006; Borrego, 2009; Mestre 2002, Redfors & Ryder, 2001).

It is surely interesting to be able to use a questionnaire as a "diagnostic instrument," i.e., to know details about relationships between student answers to the questions and what these answers might indicate about their understanding. Thereby, student reasoning lines that make explicit such an understanding, can be inferred from the student "answering strategies," i.e., the typical ways students answer the questions.

An analysis of student answers to a questionnaire can be performed by identifying homogeneous groups of students with respect to their answers to the questionnaire. However, clearly separating a sample of students into groups can be a complex operation, especially for samples composed of many students. The elements of each group must be similar to each other, while being substantially different from elements in other groups.

Cluster Analysis (CIA) is one of the methodologies used in mathematics and physics education research for this purpose. CIA, introduced in psychology by R. C. Tryon in 1939 (Tryon, 1939), is common in many fields, including information technology, biology, medicine, archaeology, econophysics and market research (Ott, 1999; Allen et al., 2013; Mantegna, 1999; Cowgill et al., 1999). However, although different CIA techniques have been already used in mathematics and physics education research (Springuel et al., 2010; Fazio et al., 2012, 2013; Battaglia & Di Paola, 2015; Di Paola et al., 2016; Battaglia et al., 2017a, 2017b & 2017c, Springuel et al., 2007), they have often not been sufficiently deepened from a theoretical point of view, or criticized by highlighting their characteristic strengths and weaknesses.

All these studies show that Cluster Analysis allows the researchers to identify groups of students whose characterisation can give information relevant for research in physics and mathematics education.

In particular, Ding & Beichner (2009) study five commonly used approaches to analyse multiple-choice test data (Classic Test Theory, Factor Analysis, Cluster Analysis, Item Response Theory and Model Analysis) and show that Cluster Analysis is a good method to classify students by their different reasoning lines. By means of Cluster Analysis, Springuel et al., (2007) analyse students' answers to open-ended questions about two-dimensional kinematics. Fazio et al., (2012, 2013) and Di Paola et al., (2016) analyse students' answers to specially designed written questionnaires using researcher-generated categories of reasoning. This is based on physics and mathematics research literature concerning students' understanding of a discipline's relevant content and their

typical reasoning lines. It is worth noting that these researchers also provided new information about unexpected differences between groups. Trigwell et al., (1999) use Cluster Analysis to ‘link’ teacher pedagogical approaches to student reasoning lines by collecting and analysing student performances.

CIA techniques (Everitt et al., 2011) are exploratory and do not require initial assumptions on student behaviour. This allows the researchers to overcome the main limits of other analysis methods based on the identification of a-priori behaviours (Brousseau, 1999). In this sense, CIA’s main point of strength is offering researchers the possibility of separating students into groups that can be characterised by common traits in their answers without any prior knowledge of what form those groups would take (Coates et al., 2012; Dayan, 1999; Sathya & Abraham, 2013).

In this contribution we discuss in detail an application of two CIA procedures on real data coming from students’ answers to an open-ended questionnaire, showing also their theoretical aspects and to what extent those are coherent with each other. Groups of students homogeneous with respect to the ways students answer a questionnaire are identified. Each group is characterised by means of the answering strategies the students deploy when facing the questionnaire and each characterisation allow us to infer the students’ lines of reasoning.

EDUCATIONAL DATA CODING

The logical steps to process data coming from student answers to an open- (or closed-) ended questionnaire are summarized in Figure 1. In the case of an open-ended questionnaire, first the researchers need to categorize the student answers, by means of an analysis that can reveal patterns, trends, and common themes emerging from them. Through comparison and discussion among researchers, these themes are then grouped into a number of “categories” (answering strategies, Brousseau, 1999) whose definition take into account, as much as possible, the words, the phrases, and the wording used by students (Chi, 1997). Such categories can be defined as the typical answering strategies put into action by the students when tackling the questionnaire questions. By using this procedure, an open-ended questionnaire actually becomes similar to a multiple choice one and a binary matrix will be built.

At the end of this phase, the whole set of answers given by students to the open-ended questionnaire is grouped into a limited number, M , of typical answers, i.e., the student answering strategies. M is obtained by adding all the answering strategies used by students when answering each question. In the case of closed-ended questions, this preliminary analysis is not needed, as the answers to each question are already “classified” in a limited number, i.e., the explicit options for the respondent to select from.

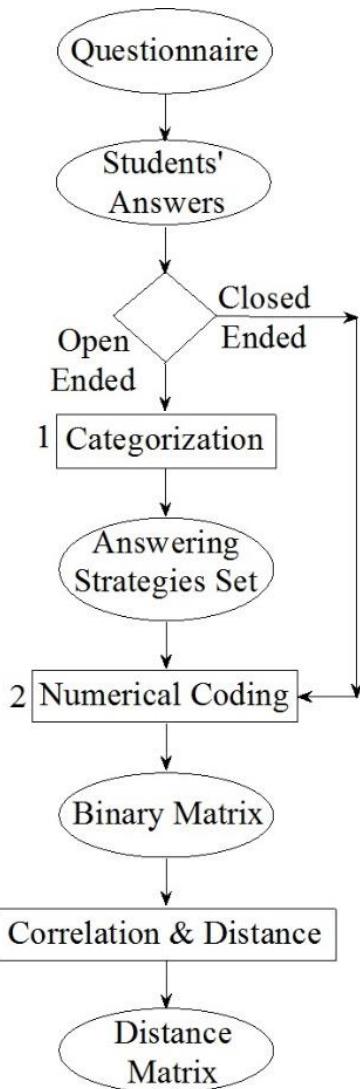


Figure 1. Flowchart of data processing for both open- and closed-ended questionnaires.

The next step, the same for both kinds of questionnaire, is the coding of the student answering strategies¹, which will generate a binary matrix. The student answering strategies can be organized in a matrix composed of 1 and 0. So, through categorization (if needed) and coding, each student, i , is identified by an array, a_i , composed of M components 1 and 0, where 1 means that the student used a given answering strategy/answering option to respond to a question and 0 means that he/she did not use it. As a consequence, an $M \times N$ binary matrix (the “matrix of answering strategies”) modelled on the one shown in Table 1, is built. The columns in it show the N student arrays, a_i , and the rows represent the M components of each array, i.e., the M answering strategies/

¹ For the sake of simplicity here we refer to the use of a two-level coding, where 1 means that a given answering strategy was used and 0 means that strategy was not used by the student.

answering options. For example, let us say that student S_1 used answering strategies AS_1 , AS_i , AS_j and AS_M to answer the questionnaire questions. Therefore, column S_1 in Table 1 will contain the binary digit 1 in the four cells corresponding to these strategies, while all the other cells will be filled with 0.

The matrix depicted in Table 1 contains all the information needed to describe the sample behaviour according to the previously described categorization. However, it needs some elaboration to be used for CIA (step 3 of Figure 1).

Table 1. Binary data matrix for N students, P questions and M answering strategies

Strategy \ Student	S_1	S_2	...	S_N
Question 1	AS_1	1	0	...

	AS_i	1	1	...
Question 2	AS_{i+1}	0	1	...
	...			
	AS_j	1	0	...
...
Question P	AS_k	0	0	...
	...			
	AS_M	1	0	...

CORRELATION AND DISTANCE

Calculations needed to perform CIA methods require the definition of new quantities like the so-called “similarity” or “distance.” These quantities are defined by starting from the $M \times N$ binary matrix discussed above and are used to build the grouping. Very often in the specialized literature (Tryon 1939, Mantegna 1999, Everitt et al., 2011) the similarity between two elements (in our case, students) i and j of a sample is discussed in terms of the distance, d_{ij} , between them (which actually expresses their “dissimilarity,” in the sense that a higher value of distance involves a lower similarity).

As we show in this section a distance can be defined by starting from the Pearson’s correlation coefficient. However, when variables are non-numerical (as in our case, where we are dealing with the arrays a_i and a_j , containing a binary coding of the answers of students i and j respectively), it cannot be used. For this reason, we introduce a new correlation coefficient, R_{bin} , similar to the one used by Tumminello et al., (2011) and Lerman (1981):

$$R_{bin}(a_i, a_j) = \frac{p(a_i \cap a_j) - \frac{p(a_i) \cdot p(a_j)}{M}}{\sqrt{p(a_i) \cdot p(a_j) \cdot \left(\frac{M-p(a_i)}{M}\right) \cdot \left(\frac{M-p(a_j)}{M}\right)}} \quad (1)$$

In eq. (1) $p(a_i)$ and $p(a_j)$ are the number of 1s in the arrays a_i and a_j , respectively, M is the total number of answering strategies and $p(a_i \cap a_j)$ is the common number of 1s in the arrays a_i and a_j . $[p(a_i) \cdot p(a_j)]/M$ is the expected value of the 1s common to a_i and a_j according to a uniform distribution.

By using eq. (1) it is possible to find $N-1$ correlation coefficients R_{bin} between each student, i , and all the others students (and the correlation coefficient with him/herself, that is, clearly, 1). All these correlation coefficients can be placed in a $N \times N$ matrix that contains the information we need to discuss the mutual relationships between our students.

The similarity between students i and j can be defined by a metric to calculate the distance d_{ij} . Such a choice depends on many factors. In our case, we assume that two students, represented by arrays a_i and a_j and negatively correlated, are more dissimilar than two uncorrelated students, so a possible definition of the distance between a_i and a_j , making use of the modified correlation coefficient, $R_{bin}(a_i, a_j)$, is:

$$d_{ij} = \sqrt{2 \cdot (1 - R_{bin}(a_i, a_j))} \quad (2)$$

This function is a Euclidean metric (Gower, 1966), which is required for the k-means algorithm. A distance d_{ij} between two students equal to zero means that they are completely similar ($R_{bin} = 1$), while a distance $d_{ij} = 2$ shows that the students are completely dissimilar ($R_{bin} = -1$). When the correlation between two students is 0 their distance is $d_{ij} = \sqrt{2}$.

By following eq. (2), we can, finally, build a new $N \times N$ matrix, \mathcal{D} (the distance matrix), containing all the mutual distances between couples of students. The main diagonal of \mathcal{D} is composed of 0s (the distance between a student and him/herself is zero). Moreover, \mathcal{D} is symmetrical with respect to the main diagonal.

K-MEANS METHOD

Clustering Analysis methods can be roughly distinguished in *Non-Hierarchical* (or *Centroid-Based*), and *Hierarchical* ones (also known as *connectivity based clustering* methods).

Non-hierarchical clustering analysis (NH-CIA) is used to generate groupings in a set of elements (in our case, students) by partitioning it and producing a smaller set of non-overlapping clusters with non-hierarchical relationships between them. Among the currently used NH-CIA algorithms, we will consider *k-means*, which was introduced by MacQueen (1963).

The result of the k-means algorithm can be graphically represented in a 2-dimensional Cartesian space. Each point is placed in the space according to the $N-1$ distances between it and the other points by using a procedure called *multidimensional scaling* (Borg & Groenen, 1997). It consists of a linear transformation between an $N-1$ dimensional vector and a 2-dimensional one, the two coordinates X and Y of the point in the Cartesian space. For this reason, the X- and Y-axes of the graph simply report the values needed to place the points expressed in arbitrary units.

The k-means algorithm starts from the choice of the number, q , of clusters one wants to populate and an equal number of “seed points.” Initially, the seed points are randomly placed in the same bi-dimensional Cartesian space, where each point represents a student. The students are then grouped on the basis of the minimum distance between themselves and the seed points. From an initial classification, students are iteratively swapped from one cluster to another and the students belonging to a given cluster are used to find a new point, representing the average position of their spatial distribution. This is done for each cluster Cl_k ($k = 1, 2, \dots, q$) and the resulting points are called the cluster *centroids* C_k . This process is repeated and ends when the new centroids coincide with the old ones. As we said above, the students, and the centroids, are finally represented in a 2-dimensional Cartesian space, creating what is known as a *k-means graph* (see, for instance, Figure 2).

Silhouette Function

The k-means algorithm has some points of weakness and here we describe how they can possibly be overcome. The first point of weakness regards the a-priori choice of the initial positions of the seed points. This is usually fixed by repeating the clustering procedure for several values of the initial conditions of seed points and selecting the result that leads to the minimum values of the distances between each centroid and the cluster elements (MacQueen, 1967; Stewart et al., 2012).

Furthermore, at the beginning of the procedure it is necessary to arbitrarily define the number, q , of clusters. A specific function, the so-called *Silhouette Function*, S , has been proposed (Rousseeuw 1987, Saxena et al., 2013) to help the researcher to decide whether this number q leads to the best clustering solution. Particularly, this function allows the researcher to decide if the partition of the sample in q clusters is adequate, how dense a cluster is, and how well a partition is differentiated from the other possible ones.

For each selected number of clusters, q , and for each sample student, i , assigned to a cluster k , with $k=1, 2, \dots, q$, a value of the *Silhouette Function*, $S_i(q)$, is calculated as

$$S_i(q) = \frac{\min_{p,p \neq k} \left(\sum_{l=1}^{N-n_k} \frac{d_{il}}{N-n_k} \right) - \sum_{j=1}^{n_k} \frac{d_{ij}}{n_k}}{\max \left[\sum_{j=1}^{n_k} \frac{d_{ij}}{n_k}, \min_{p,p \neq k} \left(\sum_{l=1}^{N-n_k} \frac{d_{il}}{N-n_k} \right) \right]} \quad (3)$$

where the first term of the numerator is the average distance of the i -th student in cluster k to l -th student placed in a different cluster p ($p = 1, \dots, q$), minimized over clusters. The second term is the average distance between the i -th student and another student j placed in the same cluster k .

Each of the $S_i(q)$ values give a measure of how similar student i is to the other students in its own cluster, when compared to students in the other ($q-1$) clusters. It ranges from -1 to +1. A value near +1 indicates that student i is well-matched to its own cluster, and poorly-matched to neighbouring clusters. If the majority of students have a silhouette value near to 1 the clustering solution is appropriate. If the silhouette values are low or negative for the majority of students then the clustering solution is not appropriate.

The values $S_i(q)$ can be averaged for each cluster k to find the average silhouette value in the cluster, $\bar{S}(q)_k$. The same can be done for the whole sample to find the total average silhouette value, $\bar{S}(q)$, for the chosen clustering solution. Large values of $\bar{S}(q)_k$ are related to the cluster elements being tightly arranged in the cluster k , and vice versa. Similarly, the larger the $\bar{S}(q)$ values, the better the clustering solutions (Rousseeuw, 1987; Saxena et al., 2013). It is, therefore, possible to perform several iterations of the cluster calculations (with different values of q) and to choose the number of clusters, q , that gives the maximum value of $\bar{S}(q)$. It has been shown (Struyf et al., 1997) that for values of $\bar{S}(q) < 0.50$, a reasonable cluster structure cannot be identified in the sample. If values are $0.51 < \bar{S}(q) < 0.70$, an acceptable cluster partition of the sample can be found. Finally, $\bar{S}(q)$ values greater than 0.70 give evidence of a strong cluster structure of the sample.

In order to exemplify the steps discussed above, we applied the k-means algorithm to a set of 150 randomly distributed elements (for instance, 150 students). Figure 2 shows the clustering results obtained by initially choosing $q = 2$ (Figure 2a), 3 (Figure 2b) and 4 (Figure 2c) as the number of clusters. The $\bar{S}(q)$ value for these three cases, 0.45, 0.47, 0.45, respectively, show that no cluster structure can be reasonably found.

Figure 3 shows the graphical representation of another set of 64 elements, again obtained on the basis of a k-means algorithm. First three clusters ($q = 3$ in Figure 3a), and then four ($q = 4$ in Figure 3b), have been chosen to start the calculations. The average silhouette values, $\bar{S}(3)$ and $\bar{S}(4)$ in this case show that a structure was found. However, $\bar{S}(3) > \bar{S}(4)$ (see also Table 2 for details on confidence intervals for the S values). This gives us evidence that, for $q = 3$, the clusters are more defined and compact than in the

second one. Moreover, in both cases $\bar{S}(3)_1$ and $\bar{S}(4)_1$ have the maximum value, showing that for both the clustering solutions cluster Cl_1 is denser and more compact than the other ones.

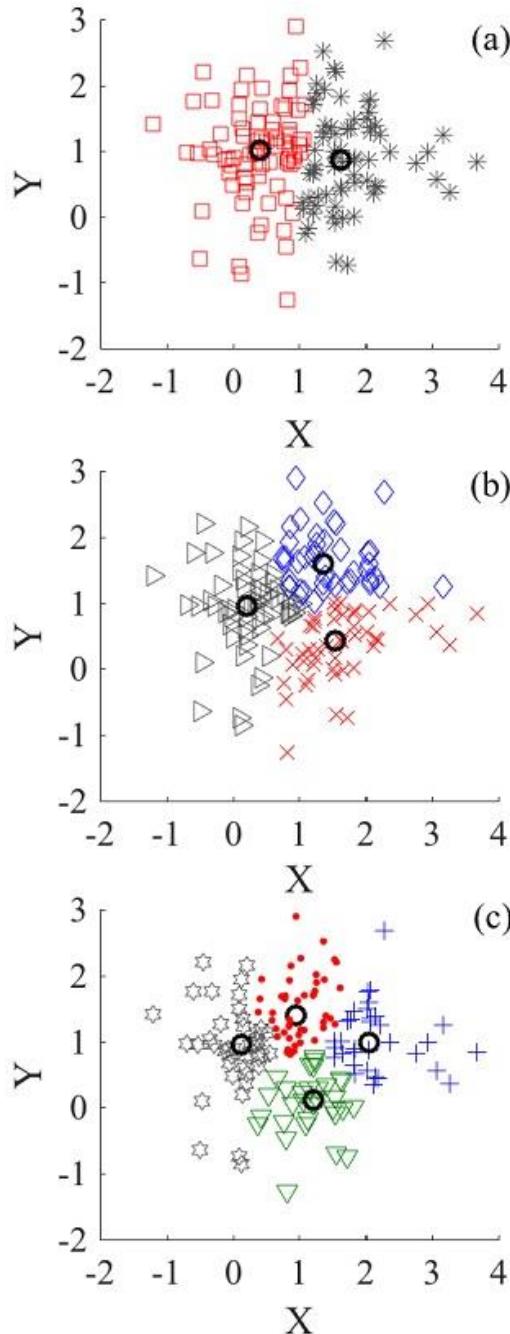


Figure 2. A randomly distributed dataset composed of 150 students partitioned in two (a), three (b) and four (c) clusters. Each point represents a student except the ones reported as black circles that are the centroids.

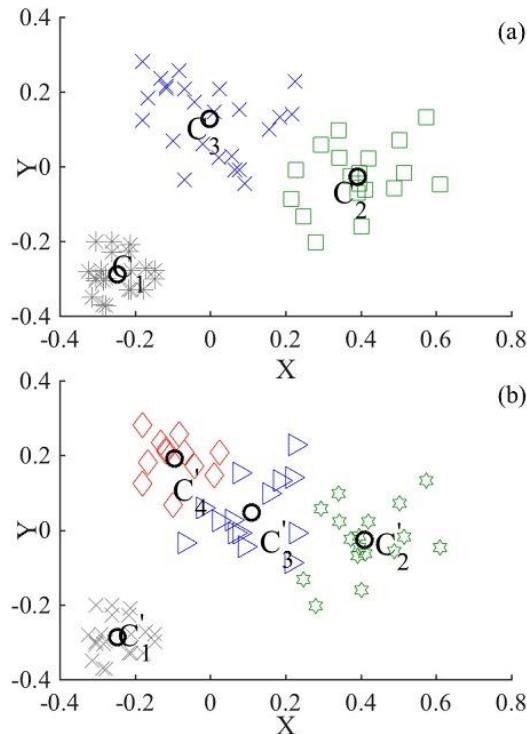


Figure 3. K-means clustering of an ad hoc built data sample composed of 64 students partitioned in three clusters (a) and in four clusters (b). Points (black circles) labelled C_1 , C_2 , C_3 , C'_1 , C'_2 , C'_3 , and C'_4 , are the centroids.

**Table 2. Silhouette values for clusters depicted in Figure 3.
The confidence intervals are reported according to a significance
level (CI) of 95%²**

q	$\bar{S}(q)$ (CI)	$\bar{S}(q)_k$ (CI)			
3	0.795 (0.780 ; 0.805)	k			
		1	2	3	
		0.953 (0.951 ; 0.956))	0.79 (0.78 ; 0.81)	0.66 (0.63 ; 0.68)	
4	0.729 (0.711 ; 0.744)	k			
		1	2	3	4
		0.953 (0.951 ; 0.956)	0.67 (0.64 ; 0.69)	0.77 (0.74 ; 0.79)	0.44 (0.40 ; 0.47)

Table 2 summarizes the silhouette values for the two different clustering solutions.

² The confidence intervals have been calculated by using the Bootstrap method (DiCiccio & Efron, 1996) as the distribution of the Silhouette values is not a-priori known.

Cluster's Characterisation

Once the appropriate partition of a given sample has been found, the researcher in education is interested in making sense of the results. This can be done by characterising each cluster in terms of the answering strategies most frequently used by the students in that cluster.

Like all the other cluster elements (the students), each centroid, C_k (with $k = 1, 2, \dots, q$) can be represented by an array, a_k^* , whose each of M components can be 0 or 1. It is worth noting that C_k has a remarkable feature. a_k^* contains 1 right in correspondence of the answering strategies most frequently used by the students in cluster k ³. A centroid is defined as the geometric point that minimizes the sum of the distances between it and all the cluster elements. By minimizing this sum, the correlation coefficients between the cluster elements and the virtual student are maximized. This happens when each virtual student has the largest number of strategies in common with the others in the same cluster.

This allows us to give meaning to the centroid as the element that characterises the cluster in the sense we discussed above.

A different way to find the array a_k^* representing the cluster k centroid starts from the coordinates of the centroid in the 2-dimensional Cartesian space reporting the results of a k-means algorithm. We devised a method that consists of repeating the *k-means* procedure in reverse, by using the iterative method described as follows. For each cluster, Cl_k , we define an array a_k^r (composed of values 1 and 0, randomly distributed) and we calculate the following value:

$$dev = \sum_i |d_{ik} - d_{ik}^r| \quad (4)$$

where d_{ik}^r is the distance between the random array and the student, i , (belonging to the same cluster Cl_k) and d_{ik} is the distance between the centroid and the same student. By using an iterative procedure that permutes the values of the random array a_k^r , we minimize the dev value and we again find that the closest array representation⁴, a_k^* , of the real centroid of C_k is 1 in correspondence of the answering strategies most frequently used by the cluster students.

From a geometric point of view it is possible to study how well a centroid characterises its cluster. Two parameters affect this: the cluster density and the number of

³ If some answering strategies are only slightly more frequent than others, all those with similar frequencies should also be considered.

⁴ As usual in a procedure to minimize an objective function (in our case, dev), the result may not be unique. In order to be sure to obtain an absolute minimum of dev , we repeated the procedure several times, each time changing the initial conditions, i.e., the random array a_k^r .

its elements.⁵ For this purpose, we propose a coefficient, r_k , defined as the centroid *reliability*. It is calculated as follows:

$$r_k = \frac{\bar{S}(q)_k}{1 - \bar{S}(q)_k} \cdot \frac{1}{n_k} \quad (5)$$

where n_k is the number of students contained in cluster Cl_k and $\bar{S}(q)_k$ is the average value of the *S-function* on the same cluster, that, as we pointed out, gives information on the cluster density.⁶ The higher the values of r_k the better the centroid characterizes the cluster.

AGGLOMERATIVE HIERARCHICAL CLUSTERING

Hierarchical clustering (H-CIA) is a method that connects elements (students in our case) to form clusters based on the presence of common characteristics. As a *hierarchy* of clusters, which merge with each other at certain distances, is provided, the term “hierarchical clustering” has been used in the specialized literature.

In H-CIA, to analyse the answers given by students to open- and closed-ended questionnaires (see, for example, (Springuel et al., 2007; Ding & Bechner, 2009; Fazio et al., 2012, 2013; Battaglia et al., 2017b), each student is initially considered as a separate cluster. Then the two ‘closest’ (the most similar) students are joined as a cluster. This process continues (in a stepwise manner) to join one student with another, a student with a cluster, or a cluster with another cluster, until all the students are combined into one single cluster as one moves up the hierarchy (*Agglomerative Hierarchical Clustering*) (Everitt et al., 2011). The results of hierarchical clustering are graphically represented as a tree, referred to as the *hierarchical tree* or *dendrogram*. The term ‘closest’ is identified by a specific rule in each of the *linkage methods*. Hence the corresponding distance matrix after each merger is differently computed in different linkage methods.

Linkage Methods

Among the many linkage methods described in the specialized literature (Everitt et al., 2011), we here discuss the following: *Single*, *Complete*, *Average* and *Weighted*

⁵ For example, two clusters with similar density but different student numbers (i.e. with different variability of student properties) are differently characterised by their centroids: the more populated cluster being less well characterised by its centroid than the other one.

⁶ The term $1 - \bar{S}(q)_k$ in (3) is needed to differently weight $\bar{S}(q)_k$ and n_k because when $\bar{S}(q)_k \rightarrow 1$ the r_k value should be independent of the value of n_k .

Average. As shown in several research fields (Springuel et al., 2007, Tumminello et al., 2011), they allow us to obtain very good clustering results that can also be easily discussed.

Each method differs in how it defines the distance between two clusters r and s . This is by means of the definition of a new metric ('ultrametric'), which consequently influences the interpretation of the word 'closest.' *Single linkage*, also called *nearest neighbour linkage*, links r and s by using the smallest distance between the students in r and those in s . *Complete linkage*, also called *farthest neighbour linkage*, uses the largest distance between the students in r and those in s . *Average linkage* uses the average distance between the students in the two clusters. Finally, *weighted average linkage* uses a recursive definition for the distance between two clusters; if cluster r was created by combining clusters p and q , the distance between r and another cluster s is defined as the average of the distance between p and s and the distance between q and s .

Table 3. "Ultrametric" distance formulas of commonly used linkages

Linkage	Ultrametric distance
Single	$\delta(r, s) = \min\{d(x_{ri}, x_{sj})\} i \in (1, \dots n_r), j \in (1, \dots n_s)$
Complete	$\delta(r, s) = \max\{d(x_{ri}, x_{sj})\} i \in (1, \dots n_r), j \in (1, \dots n_s)$
Average	$\delta(r, s) = \frac{1}{n_r n_s} \sum_i \sum_j d(x_{ri}, x_{sj})$
Weighted average	$\delta(r, s) = \frac{\delta(p, s) + \delta(q, s)}{2}$

Table 3 reports the relationships applied in order to calculate the ultrametric distances, δ , for the different linkage methods, on the basis of the Euclidean distances, d_{ij} . Supposing that r , p and q are existing clusters and cluster r is the cluster formed by merging p and q ($r = p \cup q$), the distances between the elements of r and the elements of another cluster s are defined for the four linkage methods, as shown in Table 3, where n_r indicates the number of students in cluster r , n_s indicates the number of students in cluster s , x_{ri} is the i -th student in r and x_{sj} is the j -th student in s .

To better represent the differences and approximations involved in the various linkage methods, an example is shown in Figure 4. There we report an example for a hypothetical sample of 7 elements. In this case, to better explain the meaning of different linkages, it was necessary to use a very small sample. In this way the dendrogram is easily understandable. Table 4 supplies the matrix of distances D for each couple of elements and Figures 4a, b, c and d show the four dendrograms for the single, complete,

average and weighted average linkage, respectively. The figure highlights the differences between the results obtained by using the different linkages, for example, the values of the highest linkage: $\delta = 1$ (4a), $\delta = 1.4$ (4b), $\delta = 1.08$ (4c), and $\delta = 1.2$ (4d).

Table 4. Matrix of distances of a data sample composed of 7 elements

	S1	S2	S3	S4	S5	S6	S7
S1	0	0.2	0.28	0.2	0.14	0.42	1.01
S2		0	0.2	0.28	0.14	0.42	1.01
S3			0	0.2	0.14	0.42	1.01
S4				0	0.14	0.42	1.01
S5					0	0.4	1
S6						0	1.4
S7							0

Several conditions can determine the choice of a specific linkage method. For instance, when the source data are in binary form (as in our case) the single and complete linkage methods do not give a smooth progression of the distances (Springuel et al., 2007). For this reason, when the source data are in binary form, the viable linkage methods reduce to the average or weighted average ones.

In the specialized literature it is easy to find numerical indexes driving the choice of a specific linkage method, such as the “*cophenetic correlation coefficient*” (Sokal & Sneath, 1962; Saracli et al., 2013). The cophenetic correlation coefficient, c_{coph} , gives a measure of the concordance between the two matrixes \mathcal{D} (the distances) and Δ (the ultrametric distances). It is defined as:

$$c_{coph} = \frac{\sum_{i < j} (d_{ij} - \bar{D}) \cdot (\delta_{ij} - \bar{\Delta})}{\sqrt{\sum_{i < j} (d_{ij} - \bar{D})^2 \sum_{i < j} (\delta_{ij} - \bar{\Delta})^2}} \quad (6)$$

where d_{ij} is the distance between elements i and j in \mathcal{D} , δ_{ij} is the ultrametric distance between elements i and j in Δ (i.e., the height of the link at which the two elements i and j are first joined together), and \bar{D} and $\bar{\Delta}$ are the average of \mathcal{D} and Δ , respectively.

Values of c_{coph} near to 1 indicate that the matrix Δ is actually representative of matrix \mathcal{D} and, consequently, ultrametric distances, δ_{ij} , are representative of distances, d_{ij} . Its value is based on the correlation (like the Pearson one (Springuel 2010) between the original distances, in \mathcal{D} , and the ultrametric distances given by the linkage type (contained in a new matrix, Δ). It evaluates how much the latter are actually representative of the former. More precisely, the cophenetic coefficient is a measure of how faithfully a dendrogram preserves the pair wise distances of the matrix \mathcal{D} .

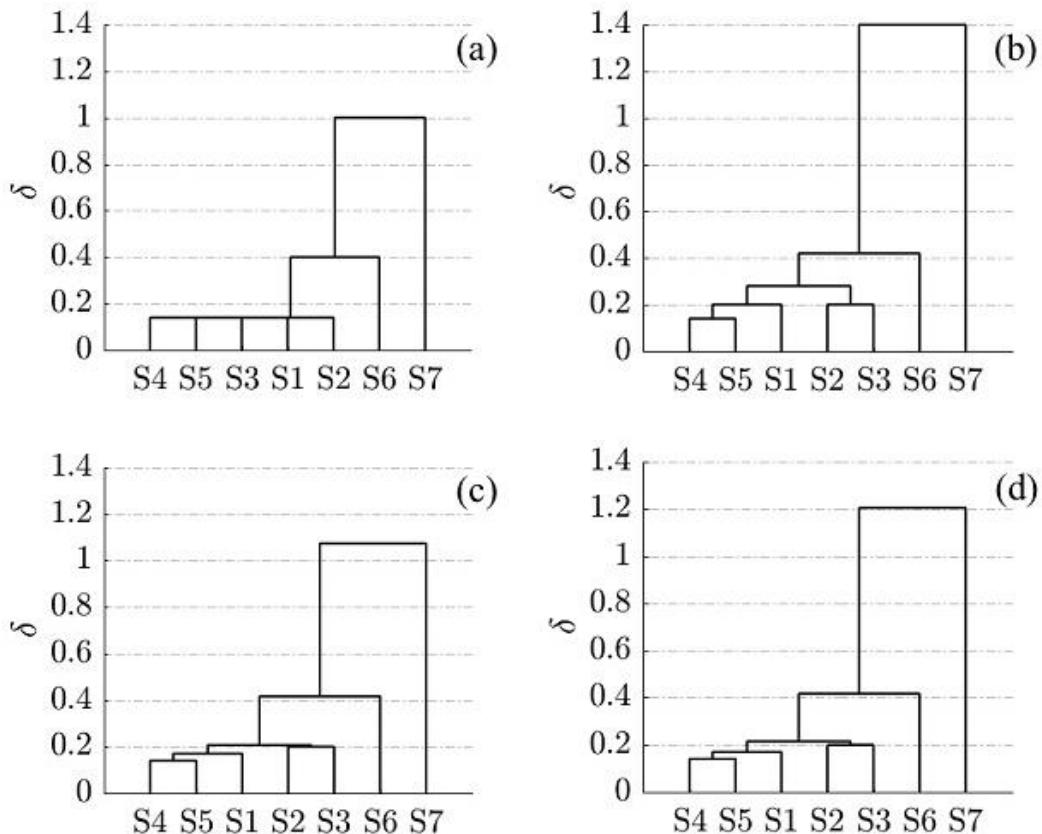


Figure 4. Dendograms obtained for single linkage (a), complete linkage (b), average linkage (c) and weighted linkage (d) for a data sample composed of 7 elements whose distances are reported in Table 4. The δ values on the Y-axis are the ‘ultrametric’ distance.

Stopping Criteria

There is no widely accepted criterion that can be applied in order to determine the best clustering solution in a dendrogram. Different criteria, named *stopping criteria*, are discussed in the specialized literature (see, for example, Springuel, 2010). Here we discuss two criteria applicable to non-numerical data. The first one is based on the calculation of the “*inconsistency coefficient*” (Ghasemi Gol et al., 2010), the second is known as “*variation ratio criterion*” (Calinski and Harabasz, 1974).

One way to decide if the grouping in a data set is adequate is to compare the height of each link in a cluster tree with the heights of neighbouring links below it in the tree. A link that is approximately the same height as the links below it indicates that there are no distinct divisions between the objects joined at this level of the hierarchy. These links are said to exhibit a high level of consistency, because the distance between the objects being joined is approximately the same as the distances between the objects they contain. A

link whose height differs noticeably from the height of the links below it indicates that the objects joined at this level in the cluster tree are much farther apart than their components were when they were joined. This link is said to be inconsistent with the links below it.

The relative consistency of each link in a hierarchical cluster tree can be quantified through the inconsistency coefficient, I_k (Sokal & Rohlf, 1962). It compares the height of each link in a cluster tree made of N elements with the heights of neighbouring links above it in the tree. The calculations of inconsistency coefficients are performed on the matrix of the ultrametric distances, Δ , generated by the chosen linkage method.

We consider two clusters, s and t , whose distance value is reported in matrix Δ , and that converge in a new link, k , (with $k = 1, 2, \dots, N-1$). If we indicate with $\delta(k)$ the height in the dendrogram of such a link, its *inconsistency coefficient* is calculated as follows:

$$I_k = \frac{\delta(k) - \bar{\delta}(k)_n}{\sigma_n(\delta(k))} \quad (7)$$

where $\delta(k)$ is the heights of the link k , $\bar{\delta}(k)_n$ is the mean of the heights of n links below the link k (usually $n = 3$ links are taken into account), and $\sigma_n(\delta(k))$ is the standard deviation of the heights of such n links.

This formula shows that a link whose height differs noticeably from the height of the n links below it indicates that the objects joined at this level in the cluster tree are much farther apart from each other than their n components. Such a link has a high value of I_k . On the contrary, if the link, k , is approximately the same height as the links below it, no distinct divisions between the objects joined at this level of the hierarchy can be identified. Such a link has a low value of I_k .

The higher the value of this coefficient, the less consistent the link connecting the students. A link that joins distinct clusters has a high inconsistency coefficient; a link that joins indistinct clusters has a low inconsistency coefficient. The choice of I_k value, a threshold, above which a link can be considered inconsistent is arbitrary.

The variation ratio criterion (*VRC*) (Calinski and Harabasz 1974) is also used in the literature to define the clustering validity. For a partition of N elements in q cluster, its value is defined as:

$$VRC = \frac{BGSS}{q-1} / \frac{WGSS}{N-q} \quad (8)$$

where *WGSS* (*Within Group Squared Sum*) represents the sum of the distance squares between the elements belonging to a same cluster and *BGSS* (*Between Group Squared Sum*), defines the sum of the distance squares between elements of a given cluster group and the external ones. The larger is the *VRC* value, the better is the clustering.

It is worth noting that the number of clusters considered significant for education-focused research should also be influenced by pedagogic considerations, related to the interpretation of the clusters that are formed. It could be desirable to have a fine grain description of our sample students; however, this could make the search for common trends in the sample too complicated and, perhaps, less interesting, if too many “micro-behaviours” related to the various small clusters are found and have to be explained.

It is important to highlight that both the criteria above described should not allow a too low or too high fragmentation⁷ of the sample clusters.

AN APPLICATION ON REAL DATA

In this section, we show an application of the methods discussed above by analysing the real answers given to a questionnaire composed of 10 open-ended questions, with 72 possible answering strategies⁸. 71 students participated in the survey and completed the questionnaire.

In order to define the number, q , of clusters that best partitions our sample, the mean value of *S-function*, $\bar{S}(q)$, has been calculated for different numbers of clusters, from 2 to 10 (see Figure 5)⁹. The figure shows that the best partition of our sample is achieved by choosing four clusters, because the value $\bar{S}(q)$ is the biggest. The obtained value $\bar{S}(4) = 0.81$, with a 95% confidence interval $CI = (0.78, 0.83)$, indicates that a reasonable 4-clusters structure has been found.

Figure 6 shows the representation of this partition in a 2-dimensional graph. It shows a partition of our sample into 4 groups made up of different numbers of students.

The four clusters $Cl_k (k = 1, \dots, 4)$ can be characterised by their related centroids, C_k . They are the four points in the graph whose arrays, a_k^* , contain the answering strategies most frequently applied by students in the related clusters (see Table 5). The codes used refer to the answering strategies for the four questions, as discussed in footnote 8. Table 5 also shows the number of students in each cluster, the mean values of the *S-function* $\bar{S}(4)_k (k = 1, \dots, 4)$ for the four clusters and the reliability index r_k of their centroids.

⁷ Here, a “too low” fragmentation is intended as a situation where one or two big clusters are produced, that do not allow us to effectively describe the sample behaviour. A “too high” fragmentation means that many small clusters, containing only a few students, are produced.

⁸ So, in the following, 1A, 1B, ... represent the identified answering strategies used by students to tackle question 1; 2A, 2B, ..., are the answering strategies for question 2, and so on.

⁹ As discussed in Section III, for each value of q the clustering procedure was repeated for several values of the initial conditions. In each case, we selected the cluster solution that leads to the minimum values of the distances between each centroid and the cluster elements.

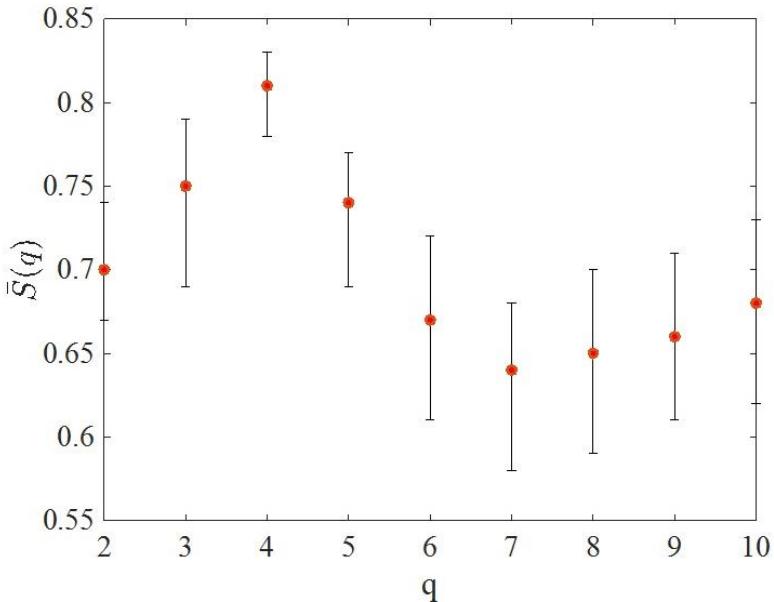


Figure 5. Average Silhouette values and related 95% confidence intervals (CI) for different clustering solutions.

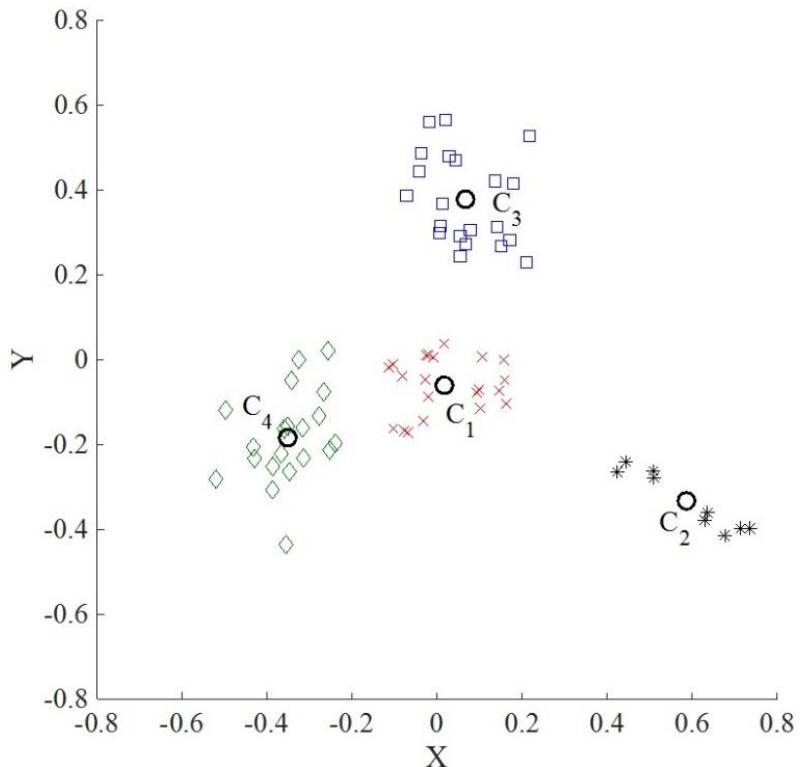


Figure 6. *k-means* graph. Each point in this Cartesian plane represents a student. Points (black circles) labelled C_1 , C_2 , C_3 , C_4 are the centroids.

Table 5. An overview of results obtained by k-means method for the 4-clusters solution

Cluster	Cl ₁	Cl ₂	Cl ₃	Cl ₄
Most frequently answers (a_k^*)	1C, 2D, 3D, 4G, 5A-F, 6A, 7C-D-F, 8E, 9F, 10F	1F-G, 2A, 3H, 4A, 5D, 6D, 7G, 9E, 10B	1B, 2B, 3D, 4G, 5A-E, 6B, 7F, 8D, 9H, 10E-F	1C, 2B, 3D, 4G, 5A-E, 6B, 7F, 8D, 9H, 10E-F
Number of students	21	9	21	20
$\bar{S}(4)_k$ k = 1,.., 4	0.80 CI = (0.74; 0.84)	0.89 CI = (0.83; 0.93)	0.81 CI = (0.76; 0.84)	0.78 CI = (0.68; 0.83)
r_k k = 1,.., 4	0.038	0.099	0.039	0.039

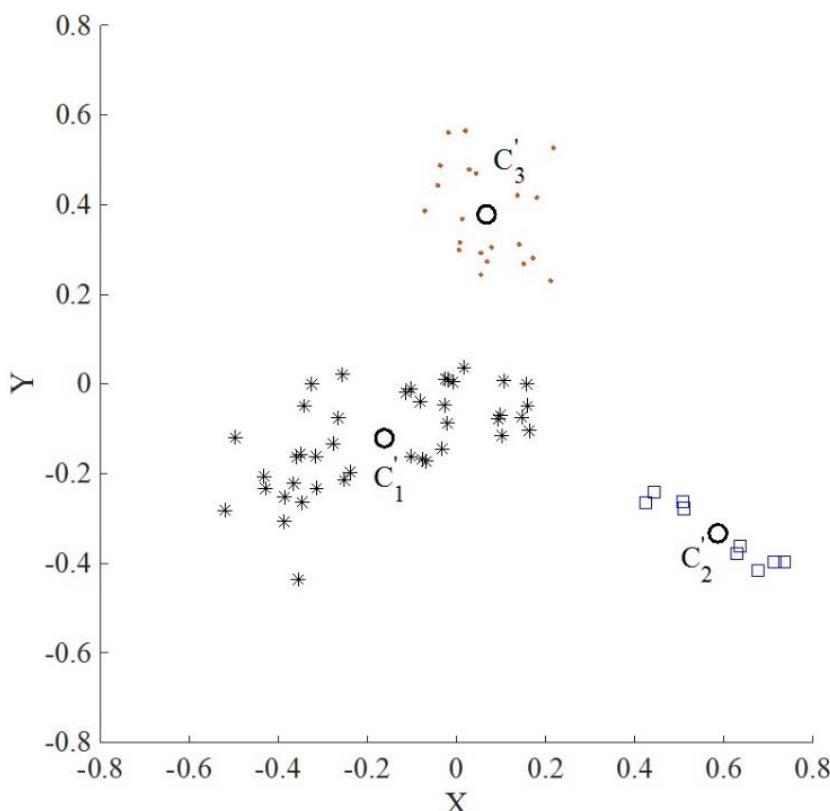


Figure 7. *k*-means graph. Each point in this Cartesian plane represents a student. Points (black circles) labelled C_1 , C_2 and C_3 are the centroids.

Table 6. An overview of results obtained by k-means method for the 3-clusters solution

Cluster	Cl ₁	Cl ₂	Cl ₃
Most frequent answers (a_k^*)	1C, 2B, 3D, 4G, 5A, 6A, 7F, 8D, 9B-H, 10F	1F-G, 2A, 3H, 4A, 5D, 6D, 7G, 9E, 10B	1B, 2B, 3D, 4G, 5A-E, 6B, 7F, 8D, 9H, 10E-F
Number of students	41	9	21
$\bar{S}(3)_k$	0.64 CI = (0.55; 0.69)	0.89 CI = (0.83; 0.93)	0.81 CI = (0.76; 0.84)
r_k	0.015	0.099	0.039

The $\bar{S}(4)_k$ value indicates that cluster Cl_2 is denser than the others, and Cl_4 is the most spread out. Furthermore, the values of r_k show that the centroid C_2 best represents its cluster, whereas C_1 is the centroid that represents its cluster the least.

However, we must not forget that a partial overlapping of the silhouette confidence intervals for clustering solutions with three and four groups has been detected (see Figure 5). This requires an analysis of the 3-clusters solution (see Figure 7), as the final choice between the two possible solutions can only be guided by educational considerations (i.e., the meaning of the solution for the researcher in education).

It is important to note that this latter solution has centroids whose components are mostly univocally identified. Conversely, in the 4-clusters solution the centroids of the clusters Cl_1 and Cl_4 differ for a few strategies. This consideration would lead us to prefer the 3-clusters solution. Once the best clustering solution has been chosen, it is the task of the researcher in education to analyse the components (the most frequent answers) of each centroid. In this way he/she can characterise the different student groups in terms of student understanding of the physical/mathematics concepts taken into account by a questionnaire.

We will now discuss the application of the *H-ClA* method to our sample. As we first have to choose what kind of linkage to use, we start by calculating the *cophenetic correlation coefficient* for different linkages. We obtain a maximum value equal to 0.84 for *average linkage*. So, we choose to use it for the analysis.

Figure 8 shows the obtained dendrogram of the nested cluster structure. In it the horizontal axis is divided into 71 ticks, each representing a student, and the vertical axis represents the ultrametric distance between two clusters when they are joined. Furthermore, vertical lines represent students or groups of students and horizontal lines represent the joining of two clusters. Vertical lines are always placed in the centre of the group of students in a cluster and horizontal lines are placed at the height corresponding to the distance between the two clusters that they join.

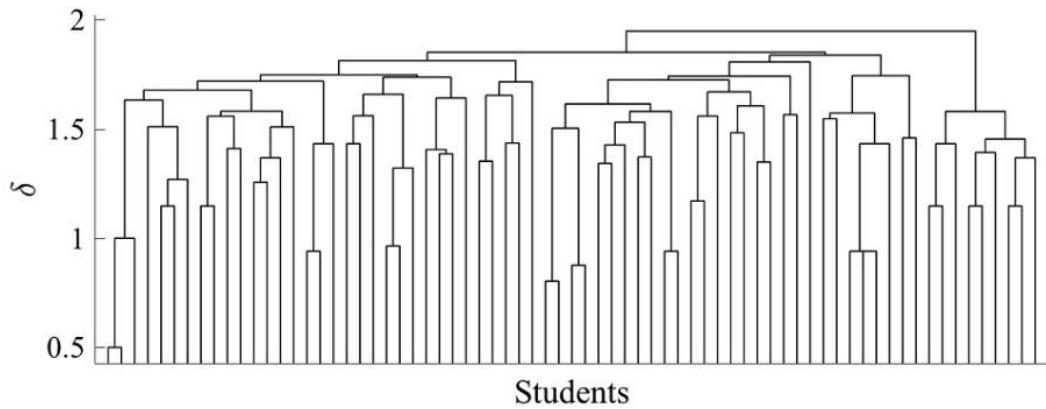


Figure 8. Dendrogram plot of our sample. Horizontal and vertical axes represent students and ultrametric distances, respectively.

By describing the cluster tree from the top down, as if clusters are splitting apart, we can see that all the students come together in a single cluster, located at the top of the figure.

In the tree shown in Figure 8 some groups of students are more closely linked and therefore we can identify clusters. In order to identify which are to be taken into account we could use the *Inconsistency Coefficient*, I_k . Unfortunately, in this case for high values of δ the values of the inconsistency coefficient are very close to each other and do not allow us to clearly discriminate the clusters.

However, if we cut the links, starting from those with the highest value of the ultrametric distance δ , we can identify different clusters. For example, by cutting the highest link, two clusters are identified.

In order to find the best partition we use the *VRC*. Table 7 shows the *VRC* values for different cluster solutions. These solutions are shown in Figures 9a - 9d.

Table 7. VRC values for different clustering solutions in the dendrogram plot

Number of clusters	Clustering solution	VRC value
2	$\alpha - \beta$	100.76
3	$\alpha - \beta_1 - \beta_2$	147.63
4	$\alpha - \beta_1 - \beta'_2 - \beta''_2$	123.71
5	$\alpha - \beta'_1 - \beta''_1 - \beta'_2 - \beta''_2$	116.42

The maximum *VRC* value is obtained for $q = 3$, corresponding to the partition $\alpha - \beta_1 - \beta_2$. This shows that the 3-cluster solution is the one that best partitions the data sample. As in the case of NH-CIA, clusters $\alpha - \beta_1 - \beta_2$ can be characterised by analysing the most frequent answers given by the students in the three clusters to each of the ten

questions in the questionnaire (see Table 8). It will be the researcher's task to inspect the most frequent answers in each cluster and their relationships, inferring the students' lines of reasoning.

We want to note here that, after having analysed the students' answers using the two different CIA methods, the researcher may find it useful to compare them. This could be done by looking at the students that are part of a cluster found by using NH methods and are also part of a cluster found by means of H methods.

Besides providing information concerning the *H-CIA* clustering results, Table 8 also allows such a comparison. By looking at the number of students, and at their identity, we can say that the 3-cluster solutions obtained by using the two Clustering methods are only slightly different, showing a good coherence.

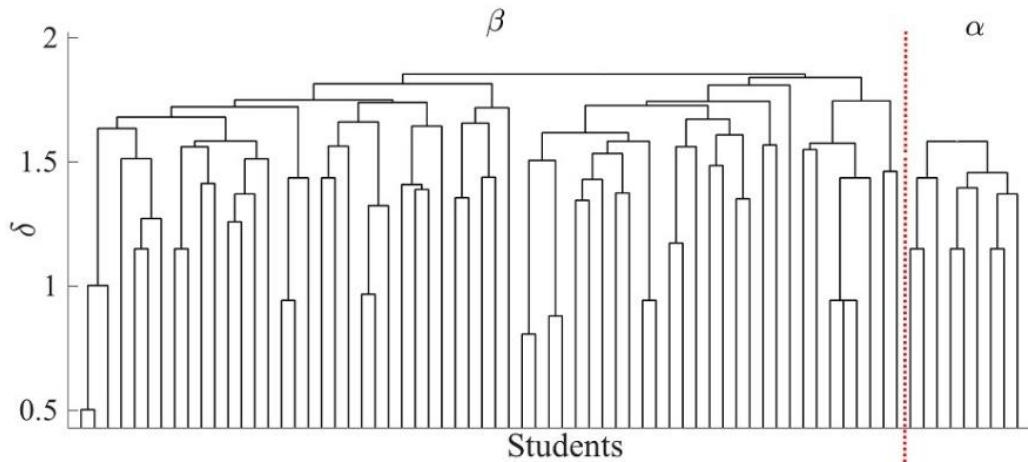


Figure 9a. 2-cluster solution. Clusters α and β are shown.

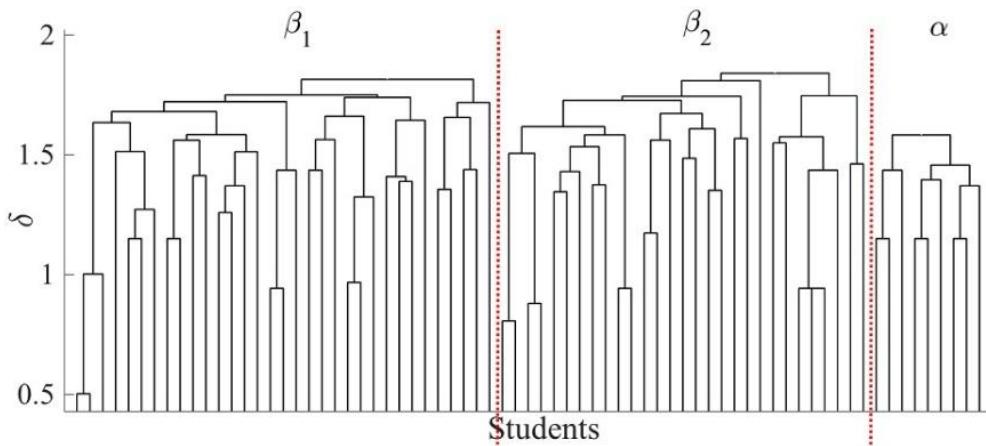


Figure 9b. 3-cluster solution. Clusters α , β_1 and β_2 are shown.

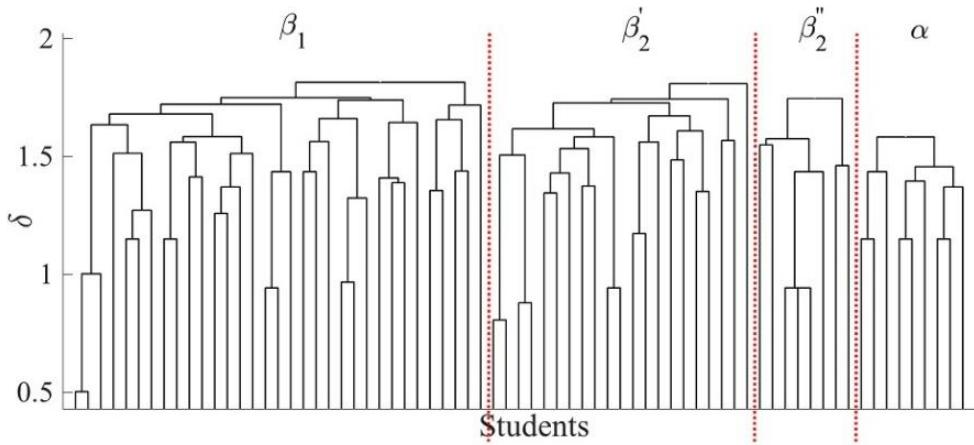


Figure 9c. 4-cluster solution. Clusters α , β_1 , β'_1 and β''_2 are shown.

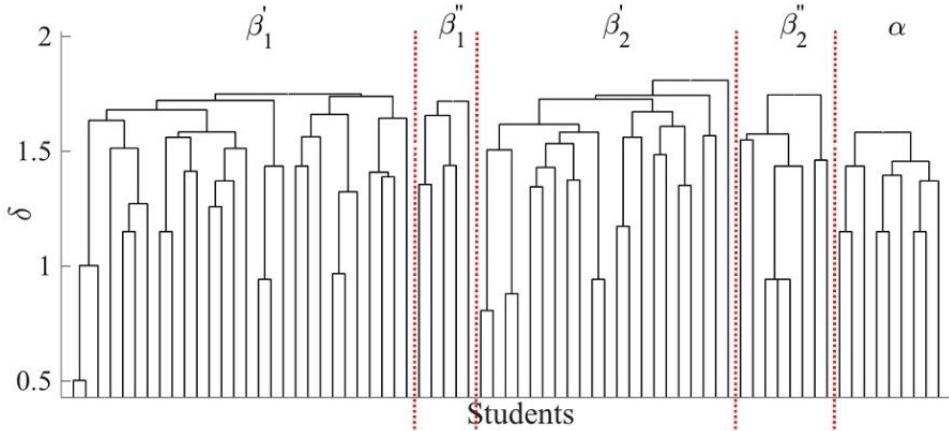


Figure 9d. 5-cluster solution. Clusters α , β'_1 , β''_1 , β'_2 and β''_2 are shown.

Table 8. An overview of results obtained by *H-ClA* and comparison with those obtained by the two previous *k-means* clustering solutions

Cluster	α	β_1	β_2
Most frequently given answers	1F-G, 2A, 3H, 4A, 5D, 6D, 7G, 9E, 10B	1C, 2B, 3D, 4G, 5A, 6A, 7F, 8D, 9B-H, 10F	1B, 2B, 3D, 4G, 5A-E, 6B, 7F, 8D, 9H, 10E-F
Number of students	9	33	29
Student distribution in the k-means clustering ¹⁰	$q = 3$ (9)Cl'_2 $q = 4$ (9)Cl_2	(33)Cl'1 (21)Cl'3+(8)Cl'1 (13)Cl_1+(20)Cl_4	(8)Cl_1+(21)Cl_3

¹⁰ i.e., (21)Cl'3+(8)Cl'1, means that cluster β_2 contains 21 students of the cluster Cl'3 (in k-means graph, 3-cluster solution) and 8 students of cluster Cl'1.

However, the specialized literature reports other ways to compare two partitions of the same data set obtained with different methods. For instance, as Meila et al., (2007, p. 891) point out: “*Just as one cannot define a “best” clustering method out of context, one cannot define a criterion for comparing clusterings that fits every problem optimally.*”

Another criterion, called *variation of information (VI)* (Meila et al., 2007), can be applied in our case. It measures the difference in information shared between two particular partitions of sample and the total information content of the two partitions. In this sense, the smaller the distance between the two clusterings, the more coherent these are with each other, and vice versa. VI can be normalized to a 0-1 range: a value equal to 0 indicates very similar clustering results, and a value equal to 1 corresponds to very different ones.

We applied this criterion to our data and calculated the value of VI to compare the 4-cluster and the 3-cluster solutions found by the *k-means* method with the 3-cluster solution of *H-CIA* method. We obtained 0.12, and 0.18, respectively. We can again conclude that the best agreement can be found between the 3-cluster solution of *k-means* algorithm and the 3-cluster solution of H-CIA method.

CONCLUSION

The use of Cluster Analysis techniques is common in many fields of research, for example, information technology, biology, medicine, archaeology, econophysics and market research. These techniques allow the researcher to locate subsets or clusters within a set of objects of any nature that have a tendency to be homogeneous ‘in some sense.’

However, only a limited number of examples of application of CIA in the field of physics and mathematics education research are available, and many aspects of the use of the various available techniques have hardly been deepened to reveal their strength and weakness points.

In this paper we discussed some theoretical aspects of two CIA methodologies and we reported an example of application on real data coming from students’ answers to an open-ended questionnaire.

We started with the problems arising from the coding procedures of student answers to closed- and open-ended questionnaires. These procedures are aimed at categorizing student answers in a limited number of ‘typical’ ways to answer each question.

A non-hierarchical CIA method, the *k-means* one, was discussed. This allowed us to separate students into groups that can be characterised by common traits in their answers to a questionnaire. Some functions and parameters useful to carefully evaluate the reliability of the results obtained have also been presented. Each of the clusters found by

the analysis can be characterised by the most frequent answers given to the questions by the students in the cluster in order to infer their reasoning lines.

Another method of analysis, based on hierarchical clustering, allowed us to visualize the clustering results in a graphic tree called ‘dendrogram’; showing the links between couples and/or groups of students on the basis of their mutual distances is also discussed. Each cluster can again be characterised on the basis of the answers most frequently given by the students in it.

We have showed that the two clustering results here discussed are coherent each other.

Both the methods can, therefore, allow the researcher to use a questionnaire as a ‘diagnostic instrument,’ establishing relationships between the students’ answering strategies and inferring what this might indicate about student understanding.

We acknowledge that this study needs deeper investigation on some relevant aspects, like the stopping criteria or the study of coherence of different clustering methods. However, we think that it could give research in mathematics and physics education a boost to further investigate the methodological aspects of different quantitative analysis methods.

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Chapter 3

INTEGRATING A COMPUTATIONAL PERSPECTIVE IN PHYSICS COURSES

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ABSTRACT

In this contribution we discuss how to develop a physics curriculum for undergraduate students that includes computing as a central element. Our contribution starts with a definition of computing and pertinent learning outcomes and assessment studies and programs. We end with a discussion on how to implement computing in various physics courses by presenting our experiences from Michigan State University in the USA and the University of Oslo in Norway.

Keywords: physics education, computational physics, computing in science education

1. INTRODUCTION

Many important recent advances in our understanding of the physical world have been driven by large-scale computational modeling and data analysis, for example, the

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2012 discovery of the Higgs boson, the 2013 Nobel Prize in chemistry for computational modeling of molecules, and the 2016 discovery of gravitational waves. Given the ubiquitous use in science and its critical importance to the future of science and engineering, scientific computing plays a central role in scientific investigations and is critical to innovation in most domains of our lives. It underpins the majority of today's technological, economic and societal feats. We have entered an era in which huge amounts of data offer enormous opportunities. By 2020, it is also expected that one out of every two jobs in the STEM (Science, Technology, Engineering and Mathematics) fields will be in computing (Association for Computing Machinery, 2013, [1]).

These developments, needs and future challenges, as well as the developments that are now taking place within quantum computing, quantum information theory and data driven discoveries (data analysis and machine learning) will play an essential role in shaping future technological developments. Most of these developments require true cross-disciplinary approaches and bridge a vast range of temporal and spatial scales and include a wide variety of physical processes. To develop computational tools for such complex systems that give physically meaningful insights requires a deep understanding of approximation theory, high performance computing, and domain specific knowledge of the area one is modeling.

Computing competence represents a central element in scientific problem solving, from basic education and research to essentially almost all advanced problems in modern societies. These competencies are not limited to STEM fields only. The statistical analysis of big data sets and how to use machine learning algorithms belong to the set of tools needed by almost all disciplines, spanning from the Social Sciences, Law, Education to the traditional STEM fields and Life Science. Unfortunately, many of our students at both the undergraduate and the graduate levels are unprepared to use computational modeling, data science, and high performance computing, skills that are much valued by a broad range of employers. This lack of preparation is most certainly no fault of our students, but rather a broader issue associated with how departments, colleges, and universities are keeping up with the demands of these high-tech employers. It is through this integrated computational perspective that we aim to address this. Furthermore, although many universities do offer compulsory programming courses in scientific computing, and physics departments offer one or more elective courses in computational physics, there is often not a uniform and coherent approach to the development of computing competencies and computational thinking. This has consequences for a systematic introduction and realization of computing skills and competencies and pertaining learning outcomes.

The aim of this contribution is to present examples on how to introduce a computational perspective in basic undergraduate physics courses, basing ourselves on experiences made at the University of Oslo in Norway and now also at Michigan State University in the USA. In particular, we will present the *Computing in Science Education*

project from the University of Oslo [2], a project which has evolved into a Center of Excellence in Education [3], the Center for Computing in Science Education. Similar initiatives and ideas are also being pursued at Michigan State University. The overarching aim is to strengthen the computing competencies of students, with key activities such as the establishment of learning outcomes, how to develop assessment programs and course transformations by including computational projects and exercises in a coherent way. The hope is that these initiatives can also lead to a better understanding of the scientific method and scientific reasoning as well as providing new and deeper insights about the underlying physics that governs a system.

This contribution is organized as follows. After these introductory remarks, we present briefly in the next section what we mean by computing and present possible learning outcomes that could be applied to a bachelor's degree program in physics (Sec. 2), which are distinguished as more general competencies and course-specific ones. In Sec. 3, we discuss possible paths on how to include and implement computational elements in central undergraduate physics courses. We discuss briefly how to assess various learning outcomes and how to develop a research program around this. Several examples that illustrate the links between the learning outcomes and specific mathematics and physics courses are discussed in Sec. 4. Finally, in the last section we present our conclusions and perspectives.

2. COMPUTING COMPETENCIES

The focus of this article is on computing competencies and how these help in enlarging the body of tools available to students and scientists alike, going well beyond classical tools taught in standard undergraduate courses in physics and mathematics. We will claim through various examples that computing allows for a more generic handling of problems, where focusing on algorithmic aspects results in deeper insights about scientific problems.

With *Computing* we will mean solving scientific problems using all possible tools, including symbolic computing, computers and numerical algorithms, experiments (often of a numerical character) and analytical paper and pencil solutions. We will thus, deliberately, avoid a discussion of computing and computational physics in particular as something separate from theoretical physics and experimental physics. It is common in the scientific literature to encounter statements like *Computational physics now represents the third leg of research alongside analytical theory and experiments*. In selected contexts where say high-performance topics or specific computational methodologies play a central role, it may be meaningful to separate analytical work from computational studies. We will however argue strongly, in particular within an educational context, for a view where computing means solving scientific problems with

all possible tools. Through various examples in this article we will show that a tight connection between standard analytical work, combined with various algorithms and a computational approach, can help in enhancing the students' understanding of the scientific method, hopefully providing deeper insights about the physics (or other disciplines). Whether and how we achieve these outcomes is the purpose of research in computational physics education.

The power of the scientific method lies in identifying a given problem as a special case of an abstract class of problems, identifying general solution methods for this class of problems, and applying a general method to the specific problem (applying means, in the case of computing, calculations by pen and paper, symbolic computing, or numerical computing by ready-made and/or self-written software).

This generic view on problems and methods is particularly important for understanding how to apply available general software to solve a particular problem. Algorithms involving pen and paper are traditionally aimed at what we often refer to as continuous models, of which only few can be solved analytically. The number of important differential equations in physics that can be solved analytically are rather few, limiting thereby the set of problems that can be addressed in order to deepen a student's insights about a particular physics case. On the other hand, the application of computers calls for approximate discrete models. Much of the development of methods for continuous models are now being replaced by methods for discrete models in science and industry, simply because we can address much larger classes of problems with discrete models, often also by simpler and more generic methodologies. In Sec. 4 we will present several examples thereof. A typical case is that where an eigenvalue problem can allow students to study the analytical solution as well as moving to an interacting quantum mechanical case where no analytical solution exists. By merely changing the diagonal matrix elements, one can solve problems that span from classical mechanics and fluid dynamics to quantum mechanics and statistical physics. Using essentially the same algorithm one can study physics cases that are covered by several courses, allowing teachers to focus more on the physical systems of interest.

There are several advantages in introducing computing in basic physics courses. It allows physics teachers to bring important elements of scientific methods at a much earlier stage in our students' education. Many advanced simulations used in physics research can easily be introduced, via various simplifications, in introductory physics courses, enhancing thereby the set of problems studied by the students (see Sec. 4). Computing gives university teachers a unique opportunity to enhance students' insights about physics and how to solve scientific problems. It gives the students the skills and abilities that are asked for by society. Computing allows for solving more realistic problems earlier and can provide an excellent training of creativity as well as enhancing the understanding of abstractions and generalizations. Furthermore, computing can decrease the need for special tricks and tedious algebra, and shifts the focus to problem

definition, visualization, and “what if” discussions. Finally, if the setup of undergraduate courses is properly designed, with a synchronization with mathematics and computational science courses, computing can trigger further insights in mathematics and other disciplines.

3. LEARNING OUTCOMES AND ASSESSMENT PROGRAMS

An essential element in designing a synchronization of computing in various physics (and other disciplines as well) courses is a proper definition of learning outcomes, as well as the development of assessment programs and possibly a pertinent research program on physics education. Having a strong physics education group that can define a proper research program is an essential part of such an endeavor. Michigan State University has a strong physics education group involved in such research programs. Similarly, the University of Oslo, with its recently established center of excellence in Education [3], has started to define a research program that aims at assessing the relevance and importance of computing in science education.

Physics, together with basic mathematics and computational science courses, is at the undergraduate level presented in a very homogeneous way worldwide. Most universities offer more or less the same topics and courses, starting with Mechanics and Classical Mechanics, Waves, Electromagnetism, Quantum physics and Quantum Mechanics and ending with Statistical physics. Similarly, during the last year of the Bachelor’s degree one finds elective courses on computational physics and mathematical methods in physics, in addition to a selection of compulsory introductory laboratory courses. Additionally, most physics undergraduate programs have now a compulsory introductory course in scientific programming offered by the computer science department. Here, one encounters frequently Python as the default programming language. Moreover, one finds almost the same topics covered by the basic mathematics courses required for a physics degree, from basic calculus to linear algebra, differential equations and real analysis. Many mathematics departments and/or computational science departments offer courses on numerical mathematics that are based on the first course in programming.

These developments have taken place during the last decade and several universities are attempting to include a more coherent computational perspective to our basic education. In order to achieve this, it is important to develop a strategy where the introduction of computational elements are properly synchronized between physics, mathematics, and computational science courses. This would allow physics teachers to focus more on the relevant physics. The development of learning outcomes plays a central role in this work. An additional benefit of properly developed learning outcomes is the stimulation of cross-department collaborations as well as an increased awareness about what is being taught in different courses. Here we list several possibilities, starting

with some basic algorithms and topics that can be taught in mathematics and computational science courses. We end with a discussion of possible learning outcomes for central undergraduate physics courses.

3.1. General Learning Outcomes for Computing Competence

Here we present some high-level learning outcomes that we expect students to achieve through comprehensive and coordinated instruction in numerical methods over the course of their undergraduate program. These learning outcomes are different from specific learning goals in that the former reference the end state that we aim for students to achieve. The latter references the specific knowledge, tools, and practices with which students should engage and discusses how we expect them to participate in that work.

Numerical algorithms form the basis for solving science and engineering problems with computers. An understanding of algorithms does not itself serve as an understanding of computing, but it is a necessary step along the path. Through comprehensive and coordinated instruction, we aim for students to have developed a deep understanding of:

- the most fundamental algorithms for linear algebra, ordinary and partial differential equations, and optimization methods;
- numerical integration including Trapezoidal and Simpson's rule, as well as multidimensional integrals;
- random numbers, random walks, probability distributions, Monte Carlo integration and Monte Carlo methods;
- root finding and interpolation methods;
- machine learning algorithms; and
- statistical data analysis and handling of data sets.

Furthermore, we aim for students to develop:

- a working knowledge of advanced algorithms and how they can be accessed in available software;
- an understanding of approximation errors and how they can present themselves in different problems; and
- the ability to apply fundamental and advanced algorithms to classical model problems as well as real-world problems as well to assess the uncertainty of their results.

Later courses should build on this foundation as much as possible. In designing learning outcomes and course contents, one should make sure that there is a progression in the use of mathematics, numerical methods and programming, as well as the contents of various physics courses. This means also that teachers in other courses do not need to use much time on numerical tools since these are naturally included in other courses.

3.1.1. Learning Outcomes for Symbolic Computing

Symbolic computing is a helpful tool for addressing certain classes of problems where a functional representation of the solution (or part of the solution) is needed. Through engaging with symbolic computing platforms, we aim for students to have developed:

- a working knowledge of at least one computer algebra system (CAS);
- the ability to apply a CAS to perform classical mathematics including calculus, linear algebra and differential equations; and
- the ability to verify the results produced by the CAS using some other means.

3.1.2. Learning Outcomes for Programming

Programming is a necessary aspect of learning computing for science and engineering. The specific languages and/or environments that students learn are less important than the nature of that learning (i.e., learning programming for the purposes of solving science problems). By numerically solving science problems, we expect students to have developed (these are possible examples):

- an understanding of programming in a high-level language (e.g., MATLAB, Python, R);
- an understanding of programming in a compiled language (e.g., Fortran, C, C++);
- the ability to implement and apply numerical algorithms in reusable software that acknowledges the generic nature of the mathematical algorithms;
- a working knowledge of basic software engineering elements including functions, classes, modules/libraries, testing procedures and frameworks, scripting for automated and reproducible experiments, documentation tools, and version control systems (e.g., Git); and
- an understanding of debugging software, e.g., as part of implementing comprehensive tests.

3.1.3. Learning Outcomes for Mathematical Modeling

Preparing a problem to be solved numerically is a critical step in making progress towards an eventual solution. By providing opportunities for students to engage in modeling, we aim for them to develop the ability to solve real problems from applied sciences by:

- deriving computational models from basic principles in physics and articulating the underlying assumptions in those models;
- constructing models with dimensionless and/or scaled forms to reduce and simplify input data; and
- interpreting the model's dimensionless and/or scaled parameters to increase their understanding of the model and its predictions.

3.1.4. Learning Outcomes for Verification

Verifying a model and the resulting outcomes it produces are essential elements in order to generate confidence in the model itself. Moreover, such verifications provide evidence that the work is reproducible. By engaging in verification practices, we aim for students to develop:

- an understanding of how to program testing procedures; and
- the knowledge of testing/verification methods including the use of:
- exact solutions of numerical models,
- classical analytical solutions including asymptotic solutions,
- computed asymptotic approximation errors (i.e., convergence rates), and
- unit tests and step-wise construction of tests to aid debugging.

3.1.5. Learning Outcomes for Presentation of Results

The results of a computation need to be communicated in some format (i.e., through figures, posters, talks, and other forms of written and oral communication). Computation affords the experience of presenting original results quite readily. Through their engagement with presentations of their findings, we aim for students to develop:

- the ability to make use of different visualization techniques for different types of computed data;
- the ability to present computed results in scientific reports and oral presentations effectively; and
- a working knowledge of the norms and practices for scientific presentations in various formats (i.e., figures, posters, talks, and written reports).

The above learning goals and outcomes are of a more generic character. What follows here are specific algorithms that occur frequently in scientific problems. The implementation of these algorithms in various physics courses, together with problem and project solving, is a way to implement large fractions of the above learning goals.

3.2. Central Tools and Programming Languages

We will strongly recommend that Python is used as the high-level programming language. Other high-level environments like Mathematica and Matlab can also be presented and offered as special courses. This means that students can apply their knowledge from the basic programming course offered by most universities. Many university courses in programming make use of Python, and extend their computational knowledge in various physics classes. We recommend that the following tools are used:

1. jupyter and ipython notebooks;
2. version control software like git and repositories like GitHub and GitLab;
3. other typesetting tools like LaTeX; and
4. unit tests and using existing tools for unit tests. Python has extensive tools for this.

The notebooks can be used to hand in exercises and projects. They can provide the students with experience in presenting their work in the form of scientific/technical reports.

Version control software allows teachers to bring in topics like making science reproducible as well as enhancing collaborative efforts among students. Using version control can also be used to help students present benchmark results, allowing others to verify their results. Unit testing is a central element in the development of numerical projects, from micro tests of code fragments, to intermediate merging of functions to final tests of the correctness of a code.

3.3. Specific Algorithms for Basic Physics Courses

For a bachelor's degree in physics, it is now more and more common to require a compulsory programming course, typically taught during the first two years of undergraduate studies. The programming course, together with mathematics courses, lay the foundation for the use of computational exercises and projects in various physics

courses. Based on this course, and the various mathematics courses included in a physics degree, there is a unique possibility to incorporate computational exercises and projects in various physics courses, without taking away the attention from the basic physics topics to be covered.

What follows below is a suggested list of possible algorithms which could be included in central physics courses. The list is by no means exhaustive and is mainly meant as a guideline of what can be included. The examples we discuss in Sec. 4, illustrate how these algorithms can be included in courses like mechanics, quantum physics/mechanics, statistical and thermal physics and electromagnetism. These are all core courses in a typical bachelor's degree in physics.

3.4. Central Algorithms

- Ordinary differential equations
 - Euler, modified Euler, Verlet and Runge-Kutta methods with applications to problems in courses on electromagnetism, methods for theoretical physics, quantum mechanics and mechanics.
- Partial differential equations
 - Diffusion in one and two dimensions (statistical physics), wave equation in one and two dimensions. These are examples of physics cases which could appear in courses on mechanics, electromagnetism, quantum mechanics, methods for theoretical physics and Laplace's and Poisson's equations in a course on electromagnetism.
- Numerical integration
 - Trapezoidal and Simpson's rule and Monte Carlo integration. Here one can envision applications in statistical physics, methods of theoretical physics, electromagnetism and quantum mechanics.
- Statistical analysis, random numbers, random walks, probability distributions, Monte Carlo integration and Metropolis algorithm. These are algorithms with important applications to statistical physics and laboratory courses.
- Linear Algebra and eigenvalue problems.
 - Gaussian elimination, LU-decomposition, eigenvalue solvers, and iterative methods like Jacobi or Gauss-Seidel for systems of linear equations. These algorithms are important for several courses, classical mechanics, methods of theoretical physics, electromagnetism and quantum mechanics.
- Signal processing

- Discrete (fast) Fourier transforms, Lagrange/spline/Fourier interpolation, numeric convolutions and circulant matrices, filtering. Here we can think of applications in electromagnetism, quantum mechanics, and experimental physics (data acquisition)
- Root finding techniques, used in methods for theoretical physics, quantum mechanics, electromagnetism and mechanics.
- Machine Learning algorithms and Statistical Data Analysis. The latter is in particular relevant for laboratory courses

In order to achieve a proper pedagogical introduction of these algorithms, it is important that students and teachers see how these algorithms are used to solve a variety of physics problems. The same algorithm, for example the solution of a second-order differential equation, can be used to solve the equations for the classical pendulum in a mechanics course or the (with a suitable change of variables) equations for a coupled RLC circuit in the electromagnetism course. Similarly, if students develop a program for studies of celestial bodies in the mechanics course, many of the elements of such a program can be reused in a molecular dynamics calculation in a course on statistical physics and thermal physics. The two-point boundary value problem for a buckling beam (discretized as an eigenvalue problem) can be reused in quantum mechanical studies of interacting electrons in oscillator traps, or just to study a particle in a box potential with varying depth and extension. We discuss some selected examples in section 4. Our coming textbook [4] will contain a more exhaustive discussion of these, combined with a more detailed list of examples and a proper discussion of learning outcomes and possible assessment programs.

In order to aid the introduction of computational exercises and projects, there is a strong need to develop educational resources. Physics is an old discipline with a large wealth of established analytical exercises and projects. In fields like mechanics, we have centuries of pedagogical developments with a strong emphasis on developing analytical skills. The majority of physics teachers are well familiar with this approach. In order to see how computing can enlarge this body of exercises and projects, and hopefully add additional insights to the physics behind various phenomena, we find it important to develop a large body of computational examples. The PICUP project, Partnership for Integration of Computation into Undergraduate physics, develops such resources for teachers and students on the integration of computational material [5]. We strongly recommend these resources.

3.4.1. Advanced Computational Physics Courses

Towards the end of undergraduate studies it is useful to offer a course which focuses on more advanced algorithms and presents compiled languages like C++ and Fortran,

languages our students will meet in actual research. Furthermore, such a course should offer more advanced projects which train the students in actual research, developing more complicated programs and working on larger projects.

3.5. Physics Education Research and Computing in Science Education

The introduction of computational elements in the various courses should be, if possible, strongly integrated with ongoing research on physics education. The Physics and Astronomy department at MSU is in a unique position due to its strong research group in physics education, the PERL group [6]. Together with the Center for Computing in Science Education at the University of Oslo [3], we are now in the process of establishing new assessments and assessment methods that address several issues associated with integrating computing into science courses. The issues include but are not limited to how well students learn computing, what new insights students gain about the specific science through computing, and how students' affective states (e.g., motivation to learn, computational self-efficacy) are affected by computing . Broadly speaking, these assessments should provide deeper insights into the integration of computing in science education in general as well as provide a structured framework for assessment of our efforts and a basis for systematic studies of student learning.

The central questions that our research must address are

1. how can we assess the effect of integrating computing into science curricula on a variety of learned-centered constructs including computational thinking, motivation, self-efficacy and science identity formation,
2. how should we structure assessments to ensure valid, reliable and impactful assessment, which provides useful information to our program and central partners, and finally
3. how can the use of these structured assessments improve student outcomes in teacher-, peer-, and self-assessment.

Addressing these questions requires a combination of qualitative techniques to construct the focus of these assessments, to build assessment items and to develop appropriate assessment methods, and quantitative techniques, including advanced statistical analysis to ensure validity and reliability of the proposed methods as well as to analyze the resulting data.

The learning objectives and learning outcomes for computational methods developed as part of the first objective form parts of the basis for the assessment program, and we will also investigate the assessment of non-content learning goals such as self-efficacy and identity formation. Identifying and investigating the role of such non-content factors will be critical to support all students in achieving our computational learning goals.

The effect of integration of computational methods into basic science courses have been sparsely studied, primarily because the practice is sparse. Further progress depends now on the development of assessments that can be used for investigative, comparative and/or longitudinal studies and to establish best practices in this emerging field. Some assessments will be developed for specific courses, but we will aim for broad applicability across institutions.

4. EXAMPLES ON HOW TO INCLUDE COMPUTING IN PHYSICS UNDERGRADUATE PROGRAMS

Having defined possible learning outcomes, we would like now to present some examples which reflect the discussions above. These examples are mainly taken from various courses at the University of Oslo, although some of them have been used at Michigan State University. Since 2003, first via the Computing in Science Education project [2] and now through the recently established center of excellence in education Center for computing in Science Education [3], computing has been introduced across disciplines in a synchronized way.

Central elements here are a compulsory programming course with a strong mathematical flavor. This course gives a solid foundation in programming as a problem solving technique in mathematics. The line of thought is that when solving mathematical problems numerically, this should enhance algorithmic thinking, and thereby the students' understanding of the scientific process. Secondly, mathematics is at least as important as before, but should be supplemented with development, analysis, implementation, verification and validation of numerical methods. Finally, these methods are used in modeling and problem solving with numerical methods and visualization, as well as traditional methods in various science courses, from the physical sciences to life science.

Crucial ingredients for the success of the computing in Science Education project has been the support from governing bodies as well as extensive cooperations across departmental boundaries. And finally, the willingness of several university teachers and researchers to give priority to teaching reforms and course transformations.

In addition to the above, over the years we have coordinated the use of computational exercises and numerical tools in most undergraduate courses. Furthermore, via the computing in Science Education project and now the Center for computing in Science Education, we help in updating the scientific staff's competence on computational aspects and give support (scientific, pedagogical and financial) to those who wish to revise their courses in a computational direction. This may include the organization of courses for university teachers. Summer students aid in developing and introducing computational exercises and several new textbooks have been developed, from the basic mechanics course to a course in statistical physics [7-9].

4.1. The Physics Undergraduate Program at the University of Oslo

The layout of the physics bachelor's degree program at the University of Oslo is shown in Table 1.

**Table 1. The bachelor's degree program in physics
at the University of Oslo, Norway**

6 th Semester	Elective	Elective	Elective
5 th Semester	FYS2160 Statistical physics	FYS3110 Quantum Mechanics	Elective
4 th Semester	FYS2130 Waves and Motion	FYS2140 Quantum physics	FYS2150 physics Laboratory
3 rd Semester	FYS1120 Electromagnetism	MAT1120 Linear Algebra	AST2000 Intro to Astrophysics
2 nd Semester	FYS-MEK1100 Mechanics	MEK1100 Vector Calculus	MAT1110 Calculus and Linear Algebra
1 st Semester	MAT 1100 Calculus	MAT-INF1100 Modeling and Computations	IN1900 Intro to Programming
Credits	10 ECTS	10 ECTS	10 ECTS

In the first semester the students encounter the first level of synchronization between computing courses and mathematics courses. As an example, consider the numerical evaluation of an integral by the trapezoidal rule. Integral calculus is typically discussed first in the calculus course MAT1100. Thereafter, the algorithm for computing the integral using the trapezoidal rule for an interval $x \in [a, b]$

$$\int_a^b f(x)dx \approx \frac{1}{2} [f(a) + 2f(a+h) + \cdots + 2f(b-h) + f(b)],$$

is discussed and developed in MAT-INF1100, the modeling and computations course that serves as an intermediate step between the standard calculus course and the programming course. Finally, the algorithm is implemented in IN1900, introduction to programming with scientific applications. We show here a typical Python code which exemplifies this.

```

from math import exp, log, sin
def Trapez(a,b,f,n):
    h = (b-a)/float(n)
    s = 0
    x = a
    for i in range(1,n,1):
        x = x+h
        s = s+ f(x)
    s = 0.5*(f(a)+f(b)) +s
    return h*s

def f1(x):
    return exp(-x*x)*log(1+x*sin(x))

a = 1; b = 3; n = 1000
result = Trapez(a,b,f1,n)
print(result)

```

Here we have defined an integral given by

$$\int_1^3 dx \exp(-x^2) \log(1 + x \sin(x))$$

Coming back to the above learning outcomes, we would like to emphasize that Python offers an extremely versatile programming environment, allowing for the inclusion of analytical studies in a numerical program. Here we show an example code with the trapezoidal rule using Python's symbolic package **Sympy** [10] to evaluate an integral and compute the absolute error with respect to the numerically evaluated one of the integral $\int_0^1 dx x^2 = 1/3$. This is shown in the following code part

```
# define x as a symbol to be used by sympy
x = Symbol('x')
exact = integrate(function(x), (x, 0.0, 1.0))
print("Sympy integration=", exact)
```

where we have defined the function to integrate in the complete Python program that follows here.

```
from math import *
from sympy import *
def Trapez(a,b,f,n):
    h = (b-a)/float(n)
    s = 0
    x = a
    for i in range(1,n,1):
        x = x+h
        s = s+ f(x)
    s = 0.5*(f(a)+f(b)) +s
    return h*s

# function to compute pi
def function(x):
    return x*x

a = 0.0; b = 1.0; n = 100
result = Trapez(a,b,function,n)
print("Trapezoidal rule=", result)
# define x as a symbol to be used by sympy
x = Symbol('x')
exact = integrate(function(x), (x, 0.0, 1.0))
print("Sympy integration=", exact)
# Find relative error
print("Relative error", abs((exact-result)/exact))
```

The following extended version of the trapezoidal rule allows us to plot the relative error by comparing with the exact result. By increasing to 10^8 points we arrive at a region where numerical errors start to accumulate, as seen in the Figure 1.

The last example shows the potential of combining numerical algorithms with symbolic calculations, allowing thereby students to validate their algorithms. With concepts like unit testing, one has the possibility to test and verify several or all parts of the code. Validation and verification are then included *naturally*.

The below example allows the student to also test the mathematical error of the algorithm for the trapezoidal rule by changing the number of integration points. The

students get trained from day one to think error analysis. Figure 1 shows clearly the region where the relative error starts increasing. The mathematical error which follows the trapezoidal rule goes as $O(h^2)$ where h is the chosen numerical step size. It is proportional to the inverse of the number of integration points n , that is $h \propto 1/n$.

Before numerical round-off errors and loss of numerical precision kick in (near $h \sim 10^{-6}$) we see that the relative error in the log-log plot has a slope which follows the mathematical error.

```

from math import log10
import numpy as np
from sympy import Symbol, integrate
import matplotlib.pyplot as plt
# function for the trapezoidal rule
def Trapez(a,b,f,n):
    h = (b-a)/float(n)
    s = 0
    x = a
    for i in range(1,n,1):
        x = x+h
        s = s+ f(x)
    s = 0.5*(f(a)+f(b)) +s
    return h*s
# function to compute pi
def function(x):
    return x*x
# define integration limits
a = 0.0; b = 1.0;
# find result from sympy
# define x as a symbol to be used by sympy
x = Symbol('x')
exact = integrate(function(x), (x, a, b))
# set up the arrays for plotting the relative error
n = np.zeros(9); y = np.zeros(9);
# find the relative error as function of integration points
for i in range(1, 8, 1):
    npts = 10**i
    result = Trapez(a,b,function,npts)
    RelativeError = abs((exact-result)/exact)
    n[i] = log10(npts); y[i] = log10(RelativeError);
plt.plot(n,y, 'ro')
plt.xlabel('n')
plt.ylabel('Relative error')
plt.show()

```

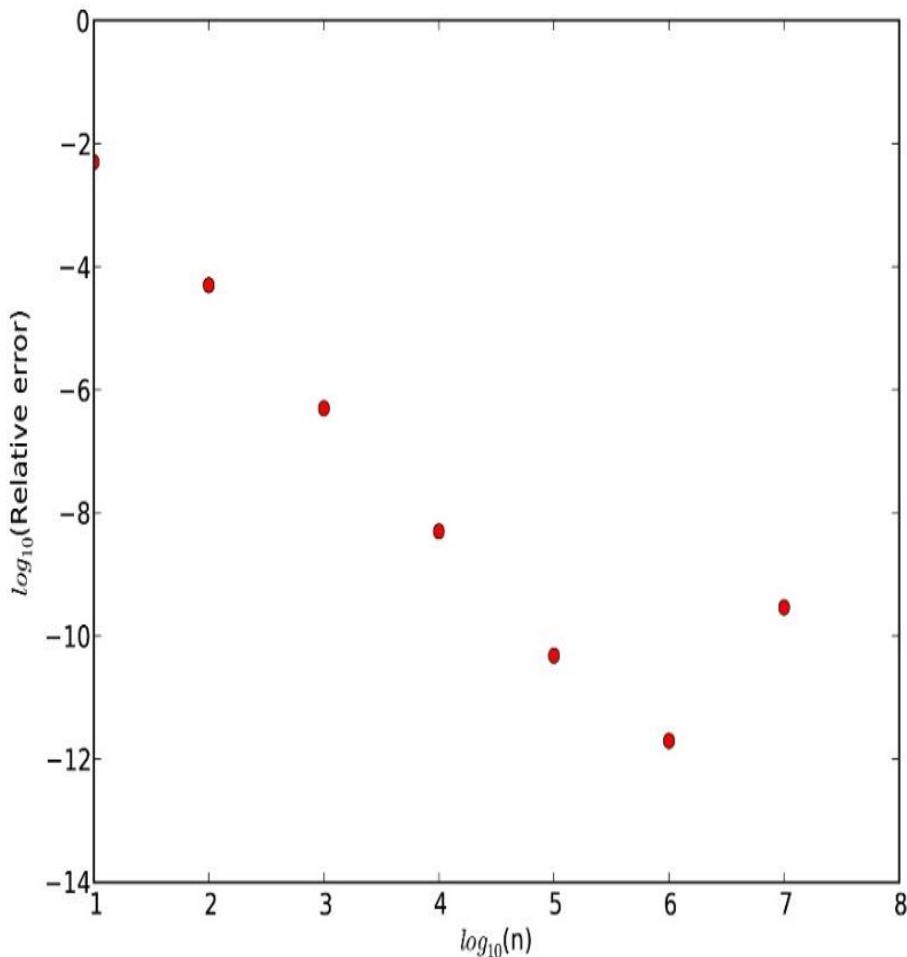


Figure 1. Log-log plot of the relative error as function of the number of integration points. Till approximately $n = 10^6$, the relative error follows the predicted mathematical error of the trapezoidal rule. For higher numbers of integration points, numerical round off errors and loss of numerical precision give an increasing relative error.

There are several additional benefits here. The general learning outcomes on computing can be included as in for example the following ways. We can easily bake in how to structure a code in terms of functions and modules, or how to read input data flexibly from the command line or how to write unit tests etc. The conventions and techniques outlined here will save students a lot of time when one extends incrementally software over time, from simpler to more complicated problems. In the next subsection we show how algorithms for solving sets of ordinary differential equations and finding eigenvalues can be reused in different courses with minor modifications only.

4.2. From Mathematics to Physics

We assume that our students know how to solve and study systems of ordinary differential with initial conditions only. Later in this section we will venture into two-point boundary value problems that can be studied and solved with eigenvalue solvers.

Let us start with initial value problems and ordinary differential equations. Such equations appear in a wealth of physics applications. Typical examples students will encounter are the classical pendulum in a mechanics course, an RLC circuit in the course on electromagnetism, the modeling of the Solar system in an Astrophysics course and many other cases. The essential message is that, with properly scaled equations, students can use essentially the same algorithms to solve these problems, either starting with a simple modified Euler algorithm or a Runge-Kutta class of algorithms or the so-called Verlet class of algorithms, to mention a few.

The idea is that algorithms students develop and use in one course can be reused in other courses. This allows students to make the relevant abstractions discussed above, opening up for a much wider range of applicabilities.

Here we look at two familiar cases from mechanics and electromagnetism, the equations for the classical pendulum and those for an RLC circuit. When properly scaled, these equations are essentially the same. To scale equations, either in terms of dimensionless variables or appropriate variables, is an important aspect which allows the students to see the potential for abstractions and hopefully see how the problems studied in say a mechanics course can be transferred to other fields.

The classical pendulum with damping and external force as it could appear in a mechanics course is given by the following equation of motion for the angle θ as function of time t

$$ml \frac{d^2\theta}{dt^2} + \nu \frac{d\theta}{dt} + mg \sin(\theta) = A \cos(\omega t),$$

where m is its mass, l the length, ν a damping factor and A the amplitude of an applied external source with frequency ω . The solution of this type of equations (second-order differential equations with given initial conditions) is something the students encounter the first semester through the courses IN1900 and MAT-INF1100 at the University of Oslo. At Michigan State University there is now a compulsory course for physics majors that includes many of these elements. With this background, students are already familiar with the numerical solution and visualization of such equations. If we now move to a course on electromagnetism, we encounter almost the same equation for an RLC circuit, namely

$$L \frac{d^2Q}{dt^2} + \frac{Q}{C} + R \frac{dQ}{dt} = A \cos(\omega t),$$

where L is the inductance, R the applied resistance, Q the time-dependent charge and C the capacitance.

Let us consider first the classical pendulum equations with damping and an external force and define the scaled velocity \hat{v} as

$$\frac{d\theta}{\hat{t}} = \hat{v},$$

where we have defined a dimensionless time variable \hat{t} . With the equation for the velocity we can rewrite the second-order differential in terms of two coupled first-order differential equations where the second equation represents the acceleration

$$\frac{d\hat{v}}{dt} = A \cos(\hat{\omega} \hat{t}) - \hat{v} \xi - \sin(\theta).$$

We have scaled the equations with $\omega_0 = \sqrt{g/l}$, $\hat{t} = \omega_0 t$ and $\xi = mg/\omega_0 v$. The frequency ω_0 defines a so-called natural frequency defined by the gravitational acceleration g and the length of the pendulum l . We have defined a dimensionless frequency $\hat{\omega} = \omega/\omega_0$. In a similar way, our RLC circuit can now be rewritten in terms of two coupled first-order differential equations,

$$\frac{dQ}{\hat{t}} = \hat{I},$$

and

$$\frac{d\hat{I}}{dt} = A \cos(\hat{\omega} \hat{t}) - \hat{I} \xi - Q,$$

with $\omega_0 = 1/\sqrt{LC}$, $\hat{t} = \omega_0 t$ and $\xi = CR\omega_0$. Here we see that the natural frequency is defined in terms of the physical parameters L and C .

The equations are essentially the same, the main differences reside in the different scaling constants and the introduction of a non-linear term for the angle θ in the pendulum equation. The differential solver the students end up writing in the mechanics course (which comes normally before the course on electromagnetism) can then be reused in the electromagnetism course, with a great potential for further abstraction.

Let us now move to another frequently encountered problem in several physics courses, namely that of a two-point boundary value problem. In the examples below we

will see again that if the equations are properly scaled, we can reuse the same algorithm for solving different physics problems. Here we will start with the equations for a buckling beam (a case which can be found in a mechanics course or a course on mathematical methods in physics). Thereafter, with a simple change of variables and constants, the same problem can be used to study a quantum mechanical particle confined to move in an infinite potential well. By simply changing the diagonal matrix elements of the discretized differential equation problem, we can study particles that move in a harmonic oscillator potential or other types of quantum-mechanical one-body or selected two-body problems. With slight modifications to the matrix that results from the discretization of a second derivative, we can study Poisson's equation in one dimension, a problem of relevance in electromagnetism.

Let us start with the buckling beam. This is a two-point boundary value problem

$$R \frac{d^2 u(x)}{dx^2} = -Fu(x),$$

where $u(x)$ is the vertical displacement, R is a material specific constant, F is the applied force and $x \in [0, L]$ with $u(0) = u(L) = 0$. We scale the equation with $x = \rho L$ and $\rho \in [0, 1]$ and get (note that we change from $u(x)$ to $v(\rho)$)

$$R \frac{d^2 v(\rho)}{d\rho^2} + Kv(\rho) = 0,$$

which is, when discretized (see below), nothing but a standard eigenvalue problem with $K = FL^2/R$. Here we can assume that either the force F or the material specific rigidity R are unknown. If we replace $R = -\hbar^2/2m$ and $-F = 2v_i$, we have the quantum mechanical variant for a particle moving in a well with infinite walls at the endpoints. The way to solve these equations numerically is to discretize the second derivative and the right hand side as

$$-\frac{v_{i+1} - 2v_i + v_{i-1}}{h^2} = \lambda v_i,$$

with $i = 1, 2, \dots, n$. Here h is the step size which is defined by the number of integration (or mesh) points. We need to add to this system the two boundary conditions $v(0) = v_0$ and $v(1) = v_{n+1}$, although they are not needed in the solution of the equations since their values are known. For all integration points the set of equations to solve result in a so-called tridiagonal Toeplitz matrix (a special case from the discretized second derivative)

$$A = \frac{1}{h^2} \begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & ... & ... & ... & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix}$$

and with the corresponding vectors $\mathbf{v} = (v_1, v_2, \dots, v_n)^T$ allows us to rewrite the differential equation as a standard eigenvalue problem

$$\mathbf{Av} = \lambda \mathbf{v}$$

The tridiagonal Toeplitz matrix has analytical eigenpairs, providing us thereby with an invaluable check on the equations to be solved.

If we stay with quantum mechanical one-body problems (or special interacting two-body problems) adding a potential along the diagonal elements allows us to reuse this problem for many types of physics cases. To see this, let us assume we are interested in the solution of the radial part of Schrödinger's equation for one electron. This equation reads

$$\frac{-\hbar^2}{2m} \left(\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} - \frac{l(l+1)}{r^2} \right) R(r) + V(r)R(r) = ER(r)$$

Suppose in our case $V(r)$ is the harmonic oscillator potential $(1/2)kr^2$ with $k = m\omega^2$ and E is the energy of the harmonic oscillator in three dimensions. The oscillator frequency is ω and the energies are

$$E_{nl} = \hbar\omega \left(2n + l + \frac{3}{2} \right),$$

with $n = 0, 1, 2, \dots$ and $l = 0, 1, 2, \dots$

Since we have made a transformation to spherical coordinates it means that $r \in [0, \infty)$. The quantum number l is the orbital momentum of the electron. In order to find analytical solutions for this problem, we would substitute $R(r) = (1/r)u(r)$ (which gives $u(0) = u(\infty) = 0$ and thereby easier boundary conditions) and obtain

$$\frac{-\hbar^2}{2m} \frac{d^2}{dr^2} u(r) \left(V(r) + \frac{l(l+1)\hbar^2}{r^2} \frac{1}{2m} \right) u(r) = Eu(r)$$

The boundary conditions are $u(0) = 0$ and $u(\infty) = 0$.

In order to scale the equations, we introduce a dimensionless variable $\rho = (1/\alpha)r$ where α is a constant with dimension length and get

$$\frac{-\hbar^2}{2m\alpha^2} \frac{d^2}{d\rho^2} v(\rho) + \left(V(\rho) + \frac{l(l+1)}{\rho^2} \frac{\hbar^2}{2m\alpha^2} \right) v(\rho) = E v(\rho)$$

Let us choose $l = 0$ for the mere sake of simplicity. Inserting $V(\rho) = (1/2)k\alpha^2\rho^2$ we end up with

$$\frac{-\hbar^2}{2m\alpha^2} \frac{d^2}{d\rho^2} v(\rho) + \frac{k}{2} \alpha^2 \rho^2 v(\rho) = E v(\rho)$$

We multiply thereafter with $2m\alpha^2/\hbar^2$ on both sides and obtain

$$\frac{d^2}{d\rho^2} v(\rho) \frac{mk}{\hbar^2} \alpha^4 \rho^2 v(\rho) + = \frac{2m\alpha^2}{\hbar^2} E v(\rho)$$

A natural length scale comes out automatically when scaling. To see this, since α is constant we are left to determine, we determine α by requiring that

$$\frac{mk}{\hbar^2} \alpha^4 = 1$$

This defines a natural length scale in terms of the various physical constants that determine the equation. The final expression, inserting $k = m\omega^2$ is

$$\alpha = \left(\frac{\hbar}{m\omega} \right)^{1/2}$$

If we were to replace the harmonic oscillator potential with the attractive Coulomb interaction from the hydrogen atom, the parameter α would equal the Bohr radius a_0 . This way students see the general properties of a two-point boundary value problem and can reuse the code they developed for a mechanics course to the subsequent quantum mechanical course.

Defining

$$\lambda = \frac{2m\alpha^2}{\hbar^2} E$$

we can rewrite Schroedinger's equation as

$$-\frac{d^2}{d\rho^2}v(\rho) + \rho^2 v(\rho) = \lambda v(\rho)$$

This is similar to the equation for a buckling beam, except for the potential term. In three dimensions with our scaling, the eigenvalues for $l = 0$ are $\lambda_0 = 3$, $\lambda_1 = 7$, $\lambda_2 = 11$,

If we define first the diagonal matrix element

$$d_i = \frac{2}{h^2} + V_i,$$

and the non-diagonal matrix element

$$e_i = -\frac{1}{h^2},$$

we can rewrite the Schröedinger equation as

$$d_i u_i + e_{i-1} v_{i-1} + e_{i+1} v_{i+1} = \lambda v_i$$

where v_i is unknown and $i = 1, 2, \dots, n$. We can reformulate the latter equation as a matrix eigenvalue problem

$$\begin{bmatrix} d_1 & e_1 & 0 & 0 & \dots & 0 & 0 \\ e_1 & d_2 & e_2 & 0 & \dots & 0 & 0 \\ 0 & e_2 & d_3 & d_3 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots & d_{n-1} & e_{n-1} \\ 0 & \dots & \dots & \dots & \dots & e_{n-1} & d_n \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ \vdots \\ v_n \end{bmatrix} = \lambda \begin{bmatrix} cv_1 \\ v_2 \\ \vdots \\ \vdots \\ v_n \end{bmatrix}$$

or if we wish to be more detailed, we can write the tridiagonal matrix as

$$\begin{bmatrix} \frac{2}{h^2} + V_1 & -\frac{1}{h^2} & 0 & 0 & \dots & 0 & 0 \\ -\frac{1}{h^2} & \frac{2}{h^2} + V_2 & -\frac{1}{h^2} & 0 & \dots & 0 & 0 \\ 0 & -\frac{1}{h^2} & \frac{2}{h^2} + V_3 & -\frac{1}{h^2} & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \dots & \frac{2}{h^2} + V_{n-1} & -\frac{1}{h^2} \\ 0 & \dots & \dots & \dots & \dots & -\frac{1}{h^2} & \frac{2}{h^2} + V_n \end{bmatrix}.$$

```

#Program which solves the one-particle Schrodinger equation
#for a potential specified in function
#potential().

from matplotlib import pyplot as plt
import numpy as np
#Function for initialization of parameters
def initialize():
    RMin = 0.0
    RMax = 10.0
    lOrbital = 0
    Dim = 400
    return RMin, RMax, lOrbital, Dim
# Harmonic oscillator potential
def potential(r):
    return 0.5*r**2

#Get the boundary, orbital momentum and number of integration points
RMin, RMax, lOrbital, Dim = initialize()

#Initialize constants
Step = RMax/(Dim)
DiagConst = 2.0/ (Step*Step)
NondiagConst = -1.0 / (Step*Step)
OrbitalFactor = lOrbital * (lOrbital + 1.0)

#Calculate array of potential values
v = np.zeros(Dim)
r = np.linspace(RMin,RMax,Dim)
for i in range(Dim):
    r[i] = RMin + (i+1) * Step;
    v[i] = potential(r[i]) + OrbitalFactor/(r[i]**2);

#Setting up a tridiagonal matrix and finding eigenvectors and eigenvalues
Matrix = np.zeros((Dim,Dim))
Matrix[0,0] = DiagConst + v[0];
Matrix[0,1] = NondiagConst;
for i in xrange(1,Dim-1):
    Matrix[i,i-1] = NondiagConst;
    Matrix[i,i] = DiagConst + v[i];
    Matrix[i,i+1] = NondiagConst;
Matrix[Dim-1,Dim-2] = NondiagConst;
Matrix[Dim-1,Dim-1] = DiagConst + v[Dim-1];
# diagonalize and obtain eigenvalues, not necessarily sorted
EigValues, EigVectors = np.linalg.eig(Matrix)
# sort eigenvectors and eigenvalues
permute = EigValues.argsort()
EigValues = EigValues[permute]
EigVectors = EigVectors[:,permute]
# now plot the results for the three lowest lying eigenstates
for i in range(3):
    print(EigValues[i])
    FirstEigvector = EigVectors[:,0]
    SecondEigvector = EigVectors[:,1]
    ThirdEigvector = EigVectors[:,2]
    plt.plot(r, FirstEigvector**2 , 'b-',r, SecondEigvector**2 , 'g-',r,
    ThirdEigvector**2 , 'r-')
    plt.axis([0,4.6,0.0, 0.025])
    plt.xlabel(r'$r$')
    plt.ylabel(r'Radial probability $r^2|R(r)|^2$')
    plt.title(r'Radial probability distributions for three lowest-lying
states')
    plt.savefig('eienvector.pdf')

```

The Python code sets up the matrix to diagonalize by defining the minimum and maximum values of r with a maximum value of integration points. It plots the eigenfunctions of the three lowest eigenstates.

The last example shows the potential of combining numerical algorithms with analytical results (or eventually symbolic calculations), allowing thereby students to test their physics understanding. One can easily switch to other potentials by simply redefining the potential function. For example, a finite box potential we have the following code example

```
# Finite depth and range box potential, with strength V
and range a
def potential(r):
    if r >= 0.0 and r <= 10.0:
        V = -0.05
    else:
        V = 0.0
```

Thereafter, the students can explore the role of the potential depth and the range of the potential. Analyzing the eigenvectors gives additional information about the spatial degrees of freedom in terms of different potentials. The possibility to visualize the results immediately, as shown in Figure 2, aids in providing students with a deeper understanding of the relevant physics.

This example contains also many of the computing learning outcomes we discussed above, in addition to those related to the physics of a particular system. We see that, by proper scaling, the students can make further abstractions and explore other physics cases easily where no analytical solutions are known. With unit testing and analytical results they can validate and verify their algorithms.

The above example allows the student to test the mathematical error of the algorithm for the eigenvalue solver by simply changing the number of integration points. Again, as discussed above in connection with the trapezoidal rule, the students get trained to develop an understanding of the error analysis and where things can go wrong. The algorithm can be tailored to any kind of one-particle problem used in quantum mechanics.

A simple rewrite allows for the reuse in linear algebra problems for solving for example Poisson's equation in electromagnetism, or the diffusion equation in one dimension. To see this and how the same matrix can be used in a course in electromagnetism, let us consider Poisson's equation. We assume that the electrostatic potential Φ is generated by a localized charge distribution $\rho(\mathbf{r})$. In three dimensions the pertinent equation reads

$$\nabla^2 \Phi = -4\pi\rho(\mathbf{r}).$$

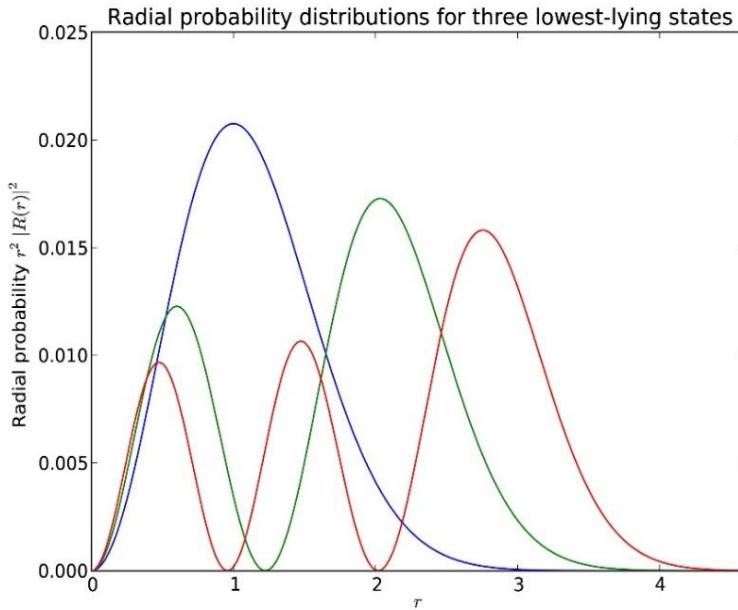


Figure 2. Plot of the Eigen functions of the three lowest-lying eigenvalues for a harmonic oscillator problem in three dimensions. The students can easily change the type of potential and explore the physics that arises from these potentials.

With a spherically symmetric potential Φ and charge distribution $\rho(\mathbf{r})$ and using spherical coordinates, the relevant equation to solve simplifies to a one-dimensional equation in r , namely

$$-\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\Phi}{dr} \right) = -4\pi\rho(r)$$

which can be rewritten via a substitution $\Phi(r) = \phi(r)/r$ as

$$\frac{d^2\phi}{dr^2} = -4\pi\rho(r)$$

The inhomogeneous term f or source term is given by the charge distribution ρ multiplied by r and the constant -4π .

We can rewrite this equation by letting $\phi \rightarrow u$ and $r \rightarrow x$. Scaling again the equations and replacing the right hand side with a function $f(x)$, we can rewrite the equation as

$$-u''(x) = f(x).$$

Our scaling gives us again $x \in [0,1]$ and the two-point boundary value problem with $u(0) = u(1) = 0$. With $n + 1$ integration points and the step length defined as $h = 1/(n)$ and replacing the continuous function u with its discretized version v , we get the following equation

$$-\frac{v_{i+1} + v_{i-1} - 2v_i}{h^2} = f_i \text{ for } i = 1, \dots, n,$$

where $f_i = f(x_i)$. Bringing up again the tridiagonal Toeplitz matrix,

$$\mathbf{A} = \frac{1}{h^2} \begin{bmatrix} 2 & -1 & 0 & \dots & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & \dots \\ 0 & -1 & 2 & -1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & -1 & 2 & -1 \\ 0 & \dots & & 0 & -1 & 2 \end{bmatrix},$$

our problem becomes now a classical linear algebra problem

$$\mathbf{Av} = \mathbf{f};$$

with the unknown function \mathbf{v} . Using standard LU decomposition algorithms [11] (here one can use the so-called Thomas algorithm which reduces the number of floating point operations to $O(n)$) one can easily find the solution to this problem.

These examples demonstrate how one can, with a discretized second derivative, solve physics problems that arise in different undergraduate courses using standard linear algebra and eigenvalue algorithms and ordinary differential equations, allowing thereby teachers to focus on the interesting physics. Many of these problems can easily be linked up with ongoing research. This opens up for many interesting perspectives in physics education. We can bring in at a much earlier stage in our education basic research elements and perhaps even link with ongoing research during the first year of undergraduate studies.

Instead of focusing on tricks and mathematical manipulations to solve the continuous problems for those few cases where an analytical solution can be found, the discretization of the continuous problem opens up for studies of many more interesting and realistic problems.

However, we have seen that in order to verify and validate our codes, the existence of analytical solutions offers us an invaluable test of our algorithms and programs. The analytical results can either be included explicitly or via symbolic software like Python's Sympy package. Thus, computing stands indeed for solving scientific problems using all

possible tools, including symbolic computing, computers and numerical algorithms, numerical experiments (as well as real experiments if possible) and analytical paper and pencil solutions.

The cases we have presented here represent only a limited set of examples. A longer version of this article, with more examples and details on assessments programs, is under preparation as a textbook [4]. The possible learning outcomes we defined for various physics courses are often based on the above simple discretization. With basic knowledge on how to solve linear algebra problems, eigenvalue problems and differential equations, topics normally taught in mathematics and computational science courses, we can offer our students a much more challenging and interesting education. Furthermore, we give our students the competencies which are required by future employers, either in the private or the public sector.

CONCLUSION AND PERSPECTIVES

In this contribution, we have outlined some of the basic elements that we feel are necessary to address in order to introduce computing in various undergraduate physics courses. Some of the conclusions we would like to emphasize include a proper definition of computing, the development of learning outcomes that apply to both computational science, mathematics, and physics courses as well as proper assessment programs.

Collaboration across departments is necessary in order to achieve a synchronization between various topics and learning outcomes, as well as an early introduction to programming. Many universities require such courses as part of a physics degree. Coordinating such a programming course with mathematics courses and other science courses results in a better coordination of both learning outcomes and computing skills and abilities. The experiences we have drawn from the University of Oslo and Michigan State University show that an early and compulsory programming course, which includes central scientific elements, is important in order to integrate properly a computational perspective in our physics education.

The benefits are many, in particular it allows us to make our research more visible in early undergraduate physics courses, enhancing research-based teaching with the possibility to focus more on understanding and increased insight. It gives also our candidates the skills and abilities that are requested by society at large, both from the private and the public sectors. With computing, we emphasize a broader and more up-to-date education with a problem-based orientation, often requested by potential employers. Furthermore, our experiences from the both universities indicate that a discussion of computing across disciplines results in an increased impetus for broad cooperation in teaching and a broader focus on university pedagogical topics.

We are now in the process of developing computing learning outcomes with examples for central physics courses. Together with a research based assessment program, we will be able to answer central questions like whether the introduction of computing increases a student's insights and understanding of the underlying physics.

ACKNOWLEDGMENTS

MHJ's work is supported by U.S. National Science Foundation Grant No. PHY-1404159. MDC's work is supported by U.S. National Science Foundation Grants Nos. DRL-1741575, DUE-1725520, DUE-1524128, DUE-1504786, and DUE-1431776. Both authors acknowledge support from the recently established Center for Computing in Science Education, University of Oslo, Norway.

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Chapter 4

LEGACY AND INFLUENCE IN MATHEMATICS AND PHYSICS WITH EDUCATIONAL TECHNOLOGY: A LABORATORY EXAMPLE

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ABSTRACT

In the last few years interdisciplinary didactics has paid increasing attention to the development of the most relevant methodology and approaches to teaching and learning. Digital tools and technology have greatly contributed to opportunities for permeable and inter-disciplinary class initiatives. The need for a shift from single subjects to the development of flexible competences within an ever-growing field of knowledge, both from a quantity and quality point of view, has emerged in the current evolution of teaching practices. This paper fits the above-mentioned theoretical framework, and puts forward an example of a laboratory with special reference to mathematical modelling through the use of technology. The authors first look at an analysis of the relationship between Mathematics and Physics, and consider a crucial aspect in the definition of such a relationship, that is, which kind of connections and integrations are needed in order to design a class initiative oriented towards the learning of interdisciplinary skills.

In particular, the authors propose a laboratory for higher secondary schools on Bréguet's spiral, a little known flat curve, which was created to guarantee a more precise functioning and performance of wrist watches. The laboratory uses computers with the aid of the dynamic geometry GeoGebra software, which allows to produce a simulation of a phenomenon of everyday life with the help of the geometrical model.

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Keywords: mathematics, physics, geometric modeling, Breguet's spiral, Lossier-Philips' curve, GeoGebra

INTRODUCTION

The connection between the understanding of Mathematics and Physics has raised the interest of international research on the teaching in the scientific-Mathematics-technology sector. Failure to recognize this association lies at the root of some of the learning difficulties experienced by students of these subjects, who indeed deem both Mathematics and Physics irksome, boring and disconnected from everyday life. It is difficult to counter this deeply rooted attitude if teachers generally carry on using communication registers and styles which are very distant from the students'. It is not only a question of the students being digital natives.

The problem lies principally in the gap between the knowledge patterns that teachers still adopt, considering them obvious, and the students' learning schemes which are strongly based on common sense and connect also to the emotional, affective and relational spheres.

In Italian secondary schools, despite the Ministry's National Guidelines¹, we can still register many cases in which the teaching of Mathematics focuses on formal narrative without conveying the true meaning and role of the subject and which still fails to link to common knowledge and with scientific and technological developments. Instead, these days school should be able to foster skills which are useful for solving problems, for separating what is of primary from what is of secondary importance, and train to identify appropriate strategies.

A teaching approach which gives students a good grounding in the field of Mathematics and Physics must necessarily make the most of the subjects' educational potential in operational learning environments derived from the real world. For example, setting up teaching initiatives on the meaning and roles of models definitely represents a good basis for the acquisition of such competences.

Also the overarching ideas established by OCSE PISA² explicitly acknowledge a great potential in the synergy between Mathematics formalization and the modelling of Physics (which involves cognitive as well as motivation aspects). Moreover, research studies have pointed out how integration and harmonization of the contents of different disciplines is a viable alternative which fosters the learning of skills [5].

¹ hubmiur.pubblica.istruzione.it/.../decreto211_7ottobre2010.doc.

² teaching-learning of Mathematics which gives emphases to proposals for problem situations set in real contexts, to research into mathematical models, and their use to solve those problems, and verifies that the chosen models are appropriate.

Alongside this, the use of technology in class has raised a lot of interest because it also helps students to tackle, from a more practical viewpoint, topics which are traditionally hard to digest [15, 19]. That is why in this delicate phase of evolution in the teaching of scientific subjects it is very appropriate to propose teaching initiatives aimed at the development of new and unexpected relations with the real world in everyday class practice.

Within this framework, the present work proposes an example of a laboratory with special reference to geometrical modelling, with the use of technology.

In practice, the authors propose a laboratorial activity for higher secondary schools on Bréguet's spiral, a little known curve, designed to give wrist watches a better and more precise performance. During the laboratory, the GeoGebra software is used specifically for the process of geometrical modelling.

In the school of the Third millennium, modelling is important because it helps us better comprehend the world around us, but also because through modelling one can acquire a flexible way of thinking which trains the mind to interpret, reflect and analyze the real world [7].

The aim is to show how Mathematics interacts with Physics and provides the conceptual tools needed to solve the problem. Mathematical modelling allows a considerable abstraction leap: the curve moves away from the subject of Physics and becomes the object of speculation and research in itself, outside the immediate applications.

THEORETICAL FRAMEWORK

In the educational process, interdisciplinary connections support a thorough comprehension of concepts and their meaning just because understanding is rooted in those associations and thus 'closed compartments' [4] can be avoided.

Senge addresses the fragmented way that we, as a culture have been trained to solve problems. He writes:

From a very early age, we are taught to break apart problems, to fragment the world. This apparently makes complex tasks and subjects more manageable, but we pay a hidden, enormous price. We can no longer see the consequences of our actions; we lose our intrinsic sense of connection to a larger whole. When we try to 'see the big picture,' we try to reassemble the fragments in our minds, to list and organize all the pieces [20, p.3].

Affirming the interdisciplinary approach means eliminating also the ‘closed compartments’ within the same discipline and enabling the students to re-use knowledge and tools in new situations to identify common grounds.

Mathematics plays a crucial role in Physics and in other fields of science and practice too. This role is brought about predominantly through the building, employment, and assessment of mathematical models. This role should also be reflected in educational settings.

Mathematics has, in fact, long been a useful language for developing Physics in a way, which is understandable for students and young people.

Modelling by mathematization specifically treats the role of Mathematics in Physics, and of the link with Mathematics in various fields of Physics education [17].

The basic elements of the existing relationship between Mathematics and Physics, revisited from the point of view of teaching implications, are the main ingredients for improving both the teaching and learning of the subjects.

This means addressing both the motivational aspects (complexity makes topics intriguing and appealing to students) and the cognitive aspects (abstract mathematical structures can be more easily understood by discussing their physical meaning; the distinction between the two could dictate the appropriate choice of register and strategies useful to overcome well known teaching and learning difficulties).

Among the connections and integrations required for the creation of integrated teaching practices between Mathematics and Physics, it is important to highlight the role of the construction model as the representation of a given phenomenon as a true knowledge experience.

As Edgard Morin says:

The aim of the cognitive activity is “to simulate” the perceived real while elaborating a mental analogon (representation), and to simulate the conceived real while elaborating an analogon idéel (theory) [18, p.109].

Therefore, analogies contribute to giving back meaning to formal objects, and offer a descriptive picture of reality which can also include an element of prediction.

The lack of coordination between the curricula of Physics and Mathematics is one of the primary causes of students’ difficulty of application of Mathematics in Physics. It is difficult for the students to transfer concepts, ideas and procedures learned in Mathematics to a new and unanticipated situation. An alternative to this traditional transfer method stresses the importance of modelling activities in an interdisciplinary context between Physics and Mathematics. Physics provides Mathematics with interesting problems to investigate, and Mathematics provides Physics with powerful tools in analyzing data and theorizing [17].

As modelling represents one of the pillars of basic scientific knowledge, it should be taken into greater consideration in the planning and managing of learning environments.

The inclusion of modelling in school Mathematics curricula is crucial for the development of problem solving skills, and promotes a reflection on the relationship between Mathematics and sensible reality [9].

A real problem offers a learning opportunity in three dimensions: familiarity with real-world problems, supporting knowledge and processes and skill [21].

From a didactic point of view, it is necessary to clarify that a model is a very distinct intellectual construction from the system it intends to represent. Also, modelling goes beyond the mere serial reproduction because it educates to an in-depth reflection on a problem; it helps to familiarize us with several important perspectives (for example, that the same mathematical model can describe different phenomena depending on the meaning of the variables) and look at well known concepts with new eyes.

Information technologies play a fundamental role in modelling and in some cases turn out to be indispensable; used in an appropriate methodological context, they help the students to capture the significance of the ‘game’ which consists in passing from the physical to the formal abstract world. In particular, the use of teaching software such as DGS (Dynamic Geometric Software) allows the simulation of the model and related affordances.

Classic heritage is transformed into information technology activities by this software, and the advantages of their use in Mathematics teaching and learning have been clearly highlighted ([3, 10, 14] and many others).

For example, in a DGS such as GeoGebra, the learner’s work differs from traditional procedures since the software allows one to experience mathematical facts directly, at different levels: the students have the real chance of creating a model and work on it constructively, exploring properties, formulating conjectures and testing them through the software tools.

The use of DGS continually opens up new didactic perspectives because it privileges the constructive aspect of the subject while at the same time maintaining the same degree of deductive accuracy, clarity of hypothesis and consequences pertaining to the discipline [11, 13, 16]. Thanks to the DGS, the graphic – constructive phase – both before the acquisition of some concepts and geometric properties, and afterwards as verification and/or in-depth analysis, greatly helps didactics, as it lends itself both to visualization and exemplification and/or exploration.

A similar process offers numerous advantages for learning the elaboration of knowledge, while at the same time teachers can throw a first glance at new learning areas that in traditional courses remain largely unexplored.

METHODOLOGY AND DESIGN OF LABORATORY

We have focused on the digital construction of the geometrical model so as to make the representation of the physical element easier (Bréguet's spiral), which enables the proper mechanical functioning of the watch. The dichotomy between the conformative³ and the representative component is of fundamental importance here.

The authors believe the representative component has greater impact on teaching, as it moves from the iconic to the semantic. The construction of the model indeed shows and communicates the synthesis between the structural composition (mechanical device) and the shape (physical element separated from the mechanism).

Centred on these considerations, the design activity is shown in Figure 1.

A historical and philosophical approach to telling the time implies a natural and coherent overlap with Physics, so we can start by introducing the idea of measuring the time, and after, lead the students to the discovery of the mechanical watch. Examination of the device through the geometrical modelling process opens the doors to Mathematics.

Thus, methodology follows the classic modelling and application process, a choice which is also supported by recent international research in the field of didactics [2, 12].

The aim is for the students to experience the object being studied, so that knowledge is acquired from both a synthesis of the processes leading to it, and the contexts in which they are used, as opposed to the acquisition of knowledge by 'closed compartments'.

Specifically, the teaching initiative begins with the introduction and analysis of the device which makes the basis for the mechanical watch, followed by a hands-on activity.

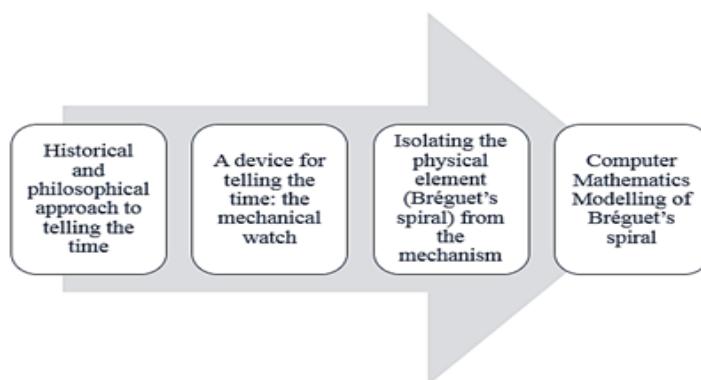


Figure 1. Design of laboratory.

In fact, at this stage the students, with the help of the teacher and the laboratory technician, disassemble the mechanical case of a clock and observe its functioning. This educational moment provides the concrete opportunity to remind the law on the

³ It goes from the reserved space to the physical element - the geometry of the mechanical device - to the volume of the wrapper (the space it occupies within another space).

isochronism of the pendulum discovered⁴ by Galileo Galilei (1564-1642) who believed that the period of oscillation of the pendulum was independent of the amplitude of the oscillations.

In reality, the students have already dealt with these contents and know perfectly, thanks to the Dutch physicist Christiaan Huygens⁵ (1629-1695), that the pendulum is strictly isochronous only if its oscillations are small in size. Naturally, the real pendulums have a tendency to dampen their motion and finally, to stop under the action of frictional forces due to the constraints and resistance of air.

At this point the teacher takes the opportunity to show the students that one of the ways in which the watchmakers solved the problem was to insert springs. In other words, the motion of the pendulum, but also of the balance in wrist watches, is guaranteed by the elastic energy accumulated by a spring which is generally spiral and wrapped around itself. The recharging of the pendulum or the mechanical clock serves to illustrate how potential elastic energy is accumulated within the spring which is wound back on itself.

Attention focuses on the different components of the ‘barrel-spiral’ system, which makes it work. Later, the ‘barrel-spiral’ system is subdivided into elements, and so the barrel spiral (Bréguet’s spiral) is isolated.

Detaching the physical element from the mechanism is the start of a process of abstraction which is at the basis of any possible interpretation; the elementary process of Mathematical modelling follows on from this, and is carried out through the use of the GeoGebra software.

So the identification of Bréguet’s spiral represents a real chance for the students to work at a deeper level, while the geometric language begins to give the object a mathematical structure.

Therefore the essence of geometry, at the same time rational and objective in its structure, is the ideal tool to use for the synthesis between the technical and scientific aspects (Bréguet’s spiral consists of 13 turns of which the first 12 are the same as Archimedes’ turns, while the last one is curved inwards).

In Euclidean geometry, the introduction of an operative phase, representative of the movement (using GeoGebra) during the various phases, leads to a structuring of the

⁴ The information related to the discovery of the isochronism and the application of the pendulum to the clock by Galileo are contained in the *Racconto istorico della vita di Galileo* [Historical account of Galileo’s life] drawn by Vincenzo Viviani (1622-1703) in the form of a letter (*Lettera di V. Viviani al Principe Leopold de’ Medici intorno all’applicazione del pendolo all’orologio*) to Prince Leopold de’ Medici (1617-1675) dated April 29 1654. Retrieved from <https://portalegalileo.museogalileo.it/egir.asp?c=300591>.

⁵ Christiaan Huygens published *Horologium oscillatorum sive de motu pendulorum ad horologia aptato demonstrationes geometricae* in Paris in 1673. This work is a general treatise on dynamics of bodies in motion, with an emphasis on the motion of the pendulum. It contains the first mathematical analysis of pendulum motion, including the formula for the relation between the period and the time of free fall from rest, the rule for deriving the center of oscillation for both simple and compound pendulums, and proof of the tautochronism of the cycloid (the arc traced by a point on a circle when the circle is rolled along a flat plane), which made possible Huygens’s invention of the first reliable pendulum clock in 1656. Retrieved from <http://www.historyofinformation.com/expanded.php?id=3044>.

actions and their effects into a descriptive framework whose convincing arguments and demonstrative clarify gradually increases.

Furthermore, the graphic representation of Bréguet's spiral offers a double advantage: it adds value to intuition on the one hand, while on the other, it allows a form of generalization, impossible with a static picture, which enables the rational handling of intuitive elements and consequently encompasses not only traditional deductive processes, but also inductive ones.

READING THE TIME

The teaching initiative starts from a broad historical and philosophical perspective so that ideas can be correctly set against an original background of discovery and novelty and in so doing, open up interdisciplinary perspectives around concepts, meanings and applications. In particular, we begin from a philosophical viewpoint with the work 'Le Confessioni di Agostino' (Augustin's Confessions), where in book eleven the question of time is taken into consideration:

Quid est ergo tempus? Si nemo ex me quaerat, scio; si quaerenti explicare velim, nescio⁶ [1, Liber XI, 16].

Augustin was the first to talk about subjective time, beginning his reflection on time from the consideration that as soon as one tries to stop it in any way, to describe it or measure it, it dissolves into nothing.

Time cannot be defined using the categories of space, because time is not *per se*, it is not something, but a relation, a reference to a system, something which is perceived by a sentient subject.

In the fourth century BC, Augustin already wonders, although not in formal terms, about the chance to measure time through prefixed units of measure⁷.

At this stage it seems appropriate to observe that time cannot be categorized, if through categories, its meanings are reorganized outside the perceiver's space.

Other philosophers and scientists have dealt with this topic, so discussion on this could be taken further.

The above considerations naturally lead us to consider now, the subject of Physics, a discipline that has greatly contributed to progress in this field by creating devices for the precise measuring of time since the beginning of history, as documented so far.

⁶ 'What is time then? If no-one asks me, I know; if I try to explain it to those that ask me, I don't know.'

⁷ How do you measure "the length of an ode from the verses, and the verses from the feet, and the feet from the length of the syllables. [...] But it may happen that a short verse, pronounced more slowly, is heard for a longer duration of time than a longer verse recited more quickly" [Augustine, XI, 26, p. 396-398].

The concept of time is obviously different from that of length; to measure the latter we can use a rigid tape measure, whereas a sample time interval can be used only once. It must be noted then that a fundamental requirement for measuring time is a ‘regular repetitive process’, as well as numerable; in other words, we must turn to a periodical process.

Watches are in fact devices (mechanical, electrical, digital, etc.), which accomplish an appropriate periodical phenomenon. At this point our attention turns to the mechanical watch that is a device made up not of a material point but of a set of objects of finite dimensions, which interact according to the laws of mechanics and are driven by forces (the spring power).

We have focused on the digital construction of the geometrical model so as to make the representation.

THE MECHANICAL WATCH

The most common mechanical watches⁸ are those to be worn on a wrist, with a barrel, anchor escapement and spring engine, the wheel work operating three hands which indicate the hour, minute and second respectively. In detail, a steel spring inside a barrel, suitably charged by the powering mechanism, represents the engine which provides the energy needed to operate the wheel work and the oscillator (Figure 2).

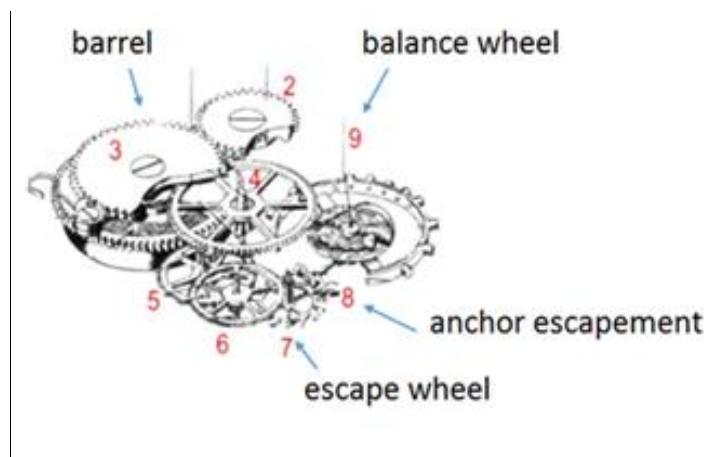


Figure 2. Mechanical watch device.

The wheel work consists of two sets of cogwheels: the main one has four coaxial wheels and as many safety pinions, each of which engages the previous wheel (“centre wheel”, whose pinion engages the barrel toothed crown, “first intermediate”, “second

⁸ Retrieved from <http://www.orologi.it/dizionario/spirale.html>.

intermediate”, ‘escape wheel’). From the axis of the centre wheel, which extends through the central hole of the face and supports the minutes hand, through a system of friction the second series of wheels depart. This comprises the demultiplier, that makes the hour hand go round and the mechanism of ‘keeping the right time’ controlled by the power button.

The observation of the mechanical device allows an initial generalization.

BREGUET’S SPIRAL

In wrist watches with a mechanical movement, time beats thanks to a spring which controls the motion of a mechanism called a balance wheel, able to oscillate on any plane. This very thin spring, coiled into a spiral shape, dictates the rhythm of the movement and regulates the marching of time thanks to its regular oscillations.

The hairspring, even though it is one the smallest components in a mechanical movement, has an essential function for the precision of the movement. It represents the heart of a watch: the central turn is fixed to the collet mounted on the axis of the balance wheel, while the external turn is fixed to the taper pin, attached to the barrel bridge (Figure 3).

The function of the hairspring is to make the barrel period uniform (making its oscillations isochronous) and with it, it forms a whole commonly called barrel-spiral system just because together they form a harmonic oscillator.

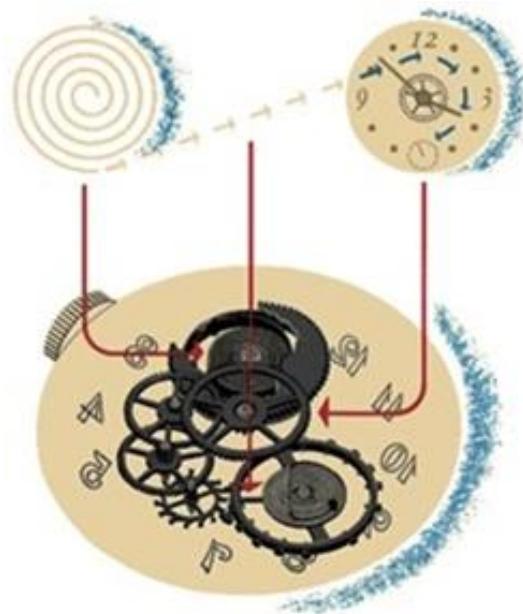


Figure 3. Barrel–spiral system.

The flat spiral was applied for the first time in 1675 by Huygens⁹. Considered as key for the accuracy of a movement, the spiral has been the object of much research, especially as far as the materials used for its construction are concerned.

For obvious reasons, isochronism of the barrel has always represented a challenge for watchmakers and designers of movements.

The key factors which interrupt such isochronism are:

- The asymmetry of the contraction and expansion of the spiral (breath);
- the varying elasticity of the spiral to variations in temperature;
- the effect of magnetic fields;
- temperature and mechanical variations at the spiral two connecting points;
- the effect of the centrifugal force and gravity on the spiral;
- inadequate dynamic balance of the barrel.

Ever since the spiral was invented, many attempts were made to eliminate these problems and Bréguet¹⁰, a famous and clever Swiss watchmaker, made a breakthrough in the history of watches both for the material used and as far as geometry was concerned.

In fact, in 1795 Bréguet modified the shape of the hairspring moving its external end towards the balance staff, following a curve (called Lossier-Phillips) calculated with mathematical precision (Figure 4). Thanks to this curve, the hairspring moves concentrically and the watch gains precision.

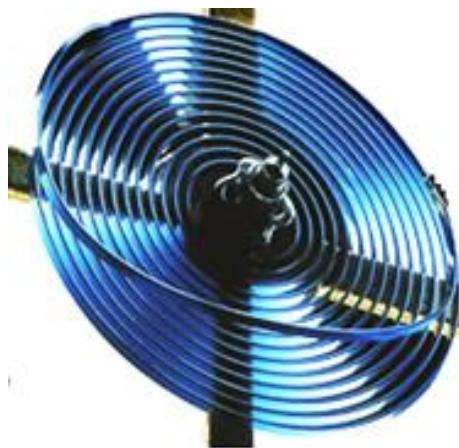


Figure 4. Bréguet's spiral.

⁹ Christian Huygens (1629-1695), Dutch mathematician and physicist, in 1675 invented the application of a concentric spiral spring which, applied to the barrel, guaranteed isochronous oscillations, and greater precision in watches as a result.

¹⁰ Abraham-Louis Breguet (1747-1823) significantly and decisively contributed to the evolution of watchmaking techniques with his inventions and technical solutions. Retrieved from <http://www.breguet.com/it/Il-Museo-Breguet>.

Compared to a classic spiral, in this new design the external turn is slightly elevated and forms an inward angle above the plane on which the rest of the spiral lies. This guarantees a better distribution of weight compared to traditional solutions, minimizing the effects of terrestrial gravity on the working of a watch.

In practice, Bréguet's spiral (Figure 4) is a spiral made up of 13 turns of which the first 12 are those of Archimedes' spiral, whereas the last turn (Lossier-Phillips' curve), is raised and bent inwards to improve isochronism.

READING THE TIME

The representative model of the barrel-spiral system as a whole provides a series of useful information on the physical significance, especially as far as the characteristics of Bréguet's spiral are concerned. At this stage of the activity, mathematical modelling enables a considerable abstraction leap: a synthetic and objective description of Bréguet's spiral requires the introduction of concepts and tools which are acquired and tested in the model study phase.

Afterwards, the evaluation of the model allows one to work to improve the tools, reflect on the theory and finally identify any further needs. So mathematical modelling, in this process, takes on the greater role of an experimenting tool with which it becomes possible to verify the mathematical properties of the curve (Figure 5).

For the reasons outlined so far, the process of modelling consists of three subsequent steps, with each step representing an improvement on the previous step. In particular, in the first step the GeoGebra spreadsheet is used like a real drawing pad by proceeding to the construction of Archimedes' spiral and the Lossier-Phillips¹¹ curve.

The second step has a strong teaching impact as it requires a sharper process of construction of the previous Archimedean spiral: the “predefined objects” contained in the GeoGebra toolbar are no longer sufficient. That is why a new tool has been designed which overcomes the problem of reiterating the process followed in the first step. The new tool is called “ArcSpiral” and aids the construction of the connected arcs of the spiral. Finally, the last step further improves the process of construction started in the previous phase and the link between the Archimedean spiral and the Lossier-Phillips' curve.

This highly formative process allows students to appreciate the potential of mathematical language while at the same time it offers a key for informed understanding of the theory.

¹¹ The construction procedure of Lossier-Phillips's curve was made on the basis of the theoretical study, that is mathematical, taken from Chapter XIII ‘La spira superiore della Bréguet's spiral’ [14, p.184-185].

The three steps are presented in detail below.

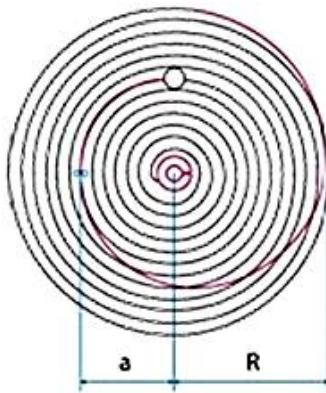


Figure 5. Drawing of Bréguet's spiral.

CONSTRUCTION OF THE BRÉGUET'S SPIRAL WITH GEOGEBRA

First Step

Classic construction of Archimedes' spiral through the “predefined objects” available in the GeoGebra toolbar: point, regular polygon, median point, half line, circumference and arc. This procedure will allow an analysis of the construction from a mathematical point of view.

Algorithm 1. Archimedes' Spiral

1. Draw two points A and B;
2. Construct the square ABCD with extreme side A and B;
3. Determine the median point (E, F, G, H) of the sides of the square;
4. Construct the rays (e, h, g, f) with origin the median point of the square and passing by one of the vertexes of the square and pertaining to the side on which the median point lies (anticlockwise direction);
5. Construct the circumference with centre A and passing by point B;
6. Determine the point of intersection I between the circumference and the ray with origin the median point of side AB and passing by A;
7. Draw the arc p with centre A and points B and I as extreme;
8. Repeat from 5 a 7:
 - a) Construct the circumference CC with centre A, B, C, D (in this order) and radius the distance between the vertex of the square and the point of

- intersection between the old circumference and the rays e, h, g, f (in this order);
- b) Construct the arc with centre in the vertex of the square.

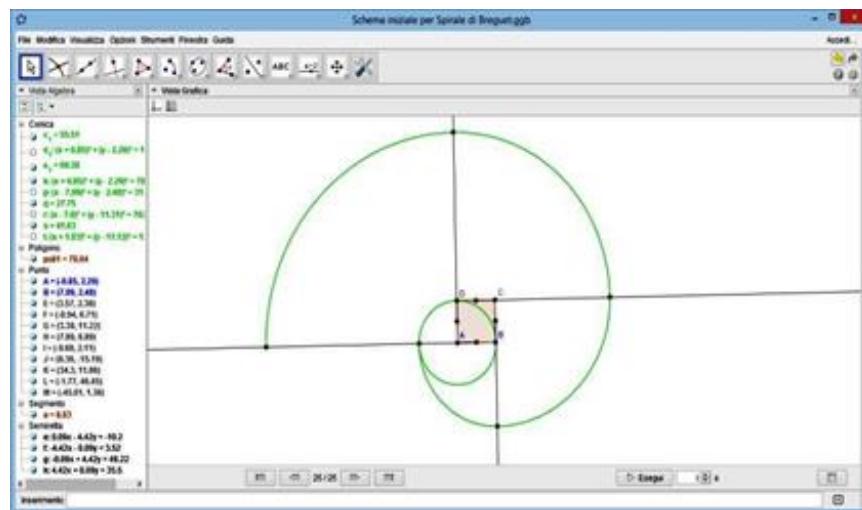


Figure 6. Output of Archimedes' spiral.

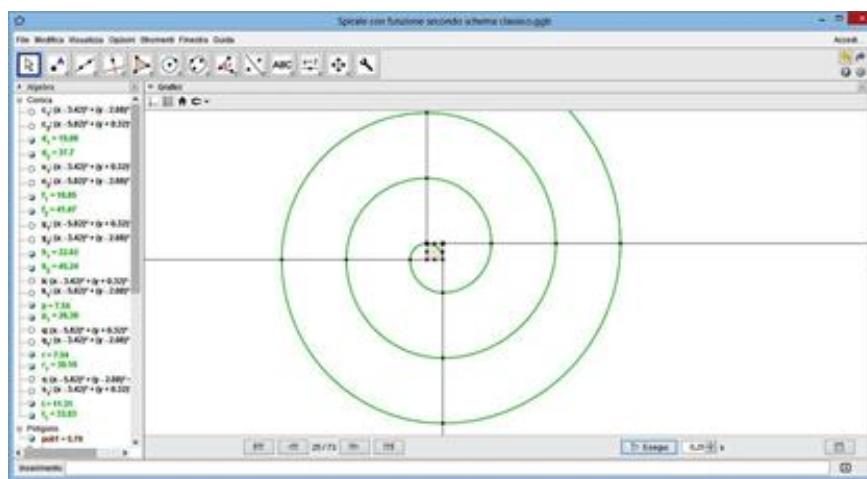


Figure 7. Partial output of Bréguet's spiral.

To complete Bréguet's spiral we must build the Lossier-Phillips' curve [6] using the tools made available by the GeoGebra spreadsheets.

Algorithm 2. Lossier – Phillips' Curve

1. Construct the circumference w with centre O and radius r (OK);
2. Allocation;

3. Draw the diameter GK;
4. Draw the point G', obtained from the rotation of point G respect to centre O by 83° angle clockwise;
5. Draw the segment OG';
6. Construct the circumference c with centre O and radius d;
7. Determine the following points of intersection: B is the point of intersection between the circumference c and the segment OG' and D is the point of intersection between the circumference c and the segment KG;
8. Draw the arc DB;
9. Construct the ray b passing by points B e O;
10. Determine the point of intersection C between the circumference w and the ray b;
11. Determine the median point A, between B and C;
12. Draw a semicircle with extremes B and C.

At the end of this phase we note how the repetition of the same “solving algorithm” takes the students to a more thorough and informed understanding of the Bréguet’s spiral.

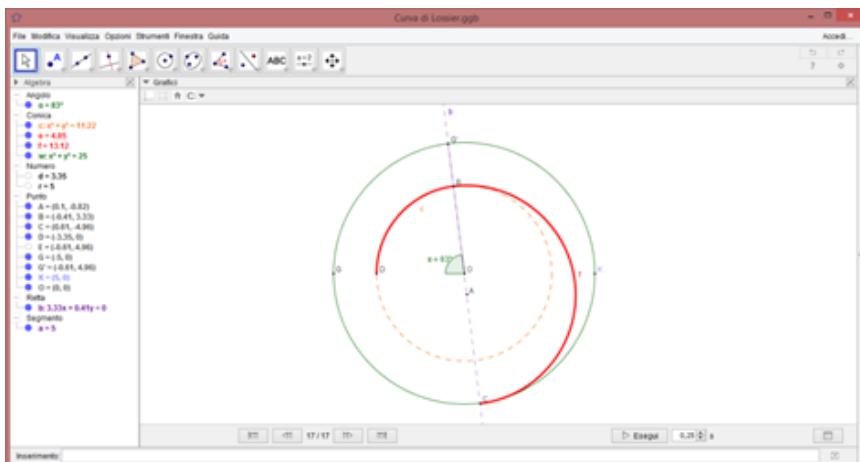


Figure 8. Output of the Lossier-Phillips' curve.

However, repeating four/five consecutive times the same algorithm may be boring, once the learners have understood that Bréguet's spiral consists of 12 complete turns (Archimedean spiral) plus a Lossier-Phillips's curve. In the Archimedean spiral, the execution of a turn requires the construction of four arcs traditionally constructed with ruler and compasses; so the need to simplify the repetition process about the construction of the connected arcs becomes apparent.

As a result, the students are asked to study a “geometrical strategy” for the solution of the problem. In this case, the GeoGebra software represents valid help as it allows the

creation of new computational tools into the spreadsheet interface, which can then be used as predefined objects.

Second Step

Design a new tool called “ArcSpiral” used for the construction of all the connected arcs so as to reduce the execution time of the previous algorithm.

This step is very sensitive because the students have to face yet another abstraction leap. They have to plan the design of a new tool called “ArcSpiral” finalized to the construction of the “ArcSpiral” tool starting from the construction of the first arc, which requires the identification of the initial objects (points A, B, median point E between A and B and the half line EA) and final (point I e arc p).

Algorithm 3: The Improved Bréguet’s Spiral

After the first seven steps of algorithm 1 we have:

1. Create a new tool “ArcSpiral”, having the points A, B and median point E between A and B, and the half line passing by points E and A as initial objects, and points I and arc p as final objects. The tool thus created can be used by clicking on its icon;
2. Construct the connected spiral arcs, through the tool “ArcSpiral”, created with appropriate choice of points.
3. Steps of algorithm 2 follow.

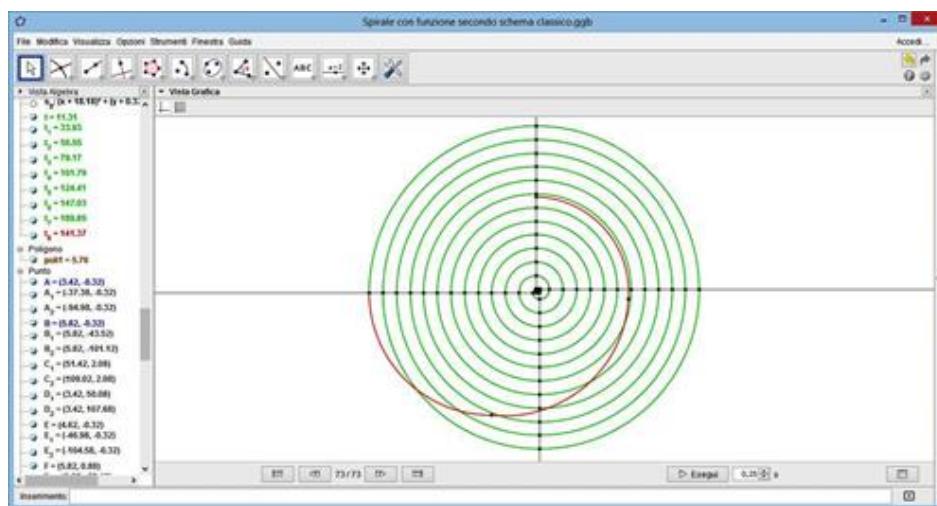


Figure 9. Final output of the complete Bréguet’s spiral.

Third Step

Design a new tool “ArcSpiral” which contains a lower number of initial objects. Planning the “ArcSpiral” tool with only two initial objects (points A and B) and one final object (arc with centre B and points A and A' as extremes).

Algorithm 4: Optimised Bréguet's Spiral

1. Draw two points A and B;
2. Draw point A', obtained from the rotation of A with respect to centre B by angle anticlockwise;
3. Construction of the arc with centre B and points A and A' as extremes;
4. Create a new tool called “Arcospiral”, with points A and B as initial objects and as final objects the arc with centre B and A and A' as extremes; the tool created can be used by clicking on its icon.

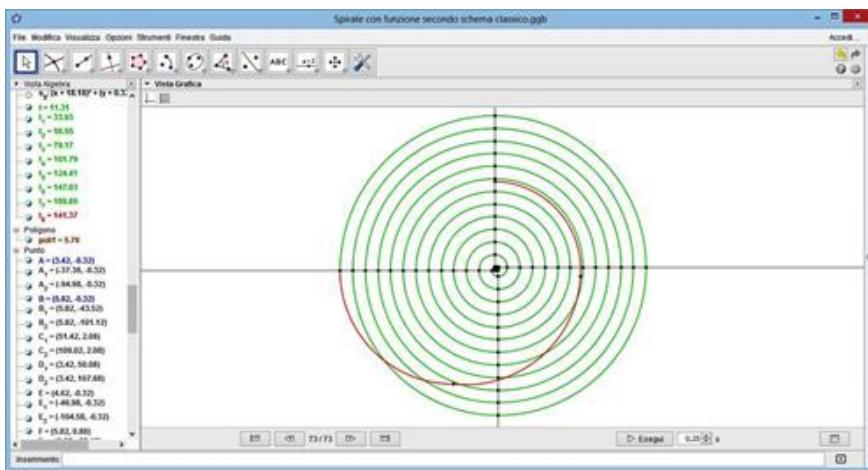


Figure 10. Output of the optimised Bréguet's spiral.

CONCLUSION

In presenting this paper the authors wish to share practices and strategies which can lead to interdisciplinary learning paths supported by an informed and innovative use of technology.

The laboratory which was set up represents an example in this direction that is an appealing and interesting educational initiative based on an open question like that of the modelling of a real situation, with the use of a representation component.

The introduction of a practical and representative dimension by means of a DSG like GeoGebra leads the students to structure the actions performed and their effects into a descriptive framework, a process through which they gradually acquire familiarity with arguments and demonstrations of increasing complexity. Moreover, the activity experience of interacting with the model is essential in order to characterize a construction and making it didactically relevant [7].

The choice of technology – the use of the GeoGebra – aids representation and communication through the symbiosis of the drawing in its phases: visualization and construction. In fact, during the different phases of geometrical modelling, GeoGebra is used as a simulation environment so as to allow the students to reproduce both the shape and the content of the Bréguet's spiral. As we know, direct experience with the model through interaction is essential to mark a simulation and make it a useful learning process.

To this end, the software is initially used at an elementary level, with direct manipulation of the available computational objects with the interface (spiral realized only by using predefined objects); then in a more and more complex and dynamic way through the design of a new tool (spiral realized with use of "ArcSpiral").

A similar refining process allows the students to test the skills they have acquired because it is based on collaboration and a motivated choice of techniques; this leads to a stronger conceptualization of Mathematics.

Furthermore, the synchronism between action and mathematics representation, that is the chance to actually see the turns as they come to 'life' makes the connection between Mathematics and Physics immediately perceptible, so this phase becomes a special opportunity for reflection on the inextricable connections between the two disciplines and on the process with which a mathematical model is constructed starting from a real physical problem.

The chosen methodology and the synergic interaction between the disciplines increases students' motivation facilitating true learning; in particular, they effectively improve the ability to formulate and solve problems, as well as demonstrate the unitariness of technical and scientific knowledge.

The proposed laboratory is innovative, though it can certainly be extended in order to go over the previous steps again in greater depth by continuous development. For example, the modelling of the curve can be done considering new criteria of representation like those of the analytical-algebraic register, etc.

Gadamer observes that the true aim of representation is to reach a truth that is allowing the recognition of something which is fixed in the real essence and that 'is free from the randomness of its appearance' [8].

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Chapter 5

EVOLUTION OF THE CONCEPT OF FORCE IN PHYSICS AND CURRENT NANOSCIENCE: NEW PERSPECTIVES IN TEACHING PROGRAMS

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ABSTRACT

Modern society requires to efficiently identify the new trends in sustainable development and their implications in future science, research and education. The recent discoveries in nanoscience and nanotechnology highlight the enhanced powerful methods of supramolecular approaches, which are based on the complex combinations of different forces acting at the molecular and supramolecular levels. These forces represent the driving interactions for the efficient assembly of building blocks, and for the creation of highly functional materials and devices with remarkable properties. The improvement of student understanding of the physical concept of force within the more broad scenery of modern nanoscience, allows a fruitful understanding of the myriad of scientific discoveries that have characterized these last years. Moreover, a major challenge in nanotechnology is the education and training of a new generation of skilled workers. Herein, a review of the evolution of the concept of force in connection with modern aspect of nanotechnology is presented. A special focus is devoted to the development of modern approaches in the academic physics programs.

Keywords: force, supramolecular structures, nanoparticles interaction, multidisciplinary teaching approaches, nanoscience and nanotechnology, physics teaching programs

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1. INTRODUCTION

The formation of graduate and post-graduate teaching programs in various field of modern science require a curriculum development oriented to the integration of modern approaches of nanoscience and nanotechnology [1, 2]. As nanoscale science and technology have an increasing impact on many aspects in our lives, the opportunities for careers are expanding rapidly. Studying science or engineering with a particular focus to the developments of modern approach of nanoscience can provide a solid foundation for a broad range of careers. European union policies has been integrating nanotechnology education in its main programs since the 2004. The European Commission Communication “towards a European strategy for nanotechnology” [3] highlighted several needs, including “promoting the interdisciplinary education and training of R&D personnel together with a stronger entrepreneurial mindset.”

The effectiveness of this policy has been strengthened by assessing numbers and types of nanotechnology curricula and courses offered in European networks and projects, and by promoting the renewal of teaching programs in universities and training institutes. In addition, the relevance of nano-education to the needs of employers has been promoted by regional programs (such as the PON programs of the European Social Fund (ESF) in Italy [4]), with particular focus on large industrial companies and small and medium enterprises (SMEs).

In this respect, the development of novel approaches and frameworks for teaching and assessing the 21st century competences in science and technology requires the joint effort to adapt traditional curriculum to the new input of modern science. Moreover, a special focus should be devoted to the development of competences and skills requested in the high technology contest of modern industries.

Herein, we review the evolution of the concept of the force, highlighting its importance in recent discoveries in the field of nanoscience and nanotechnology, with a special focus on the development of modern approaches in academic physics programs.

2. BASIC CONCEPT OF FORCE IN THE NEWTONIAN MECHANICS

The concept of force in Newtonian (or Classical) mechanics represents a central topic in the study of physics within the graduate and post-graduate programs. The classical concept of force is initially given in the three simple mechanical Newtonian laws. The second law is often regarded as a Newtonian definition of force, in which the force F is strictly connected with the concept of mass (m) and of the acceleration (a).

The basic Newtonian concept of force can be regarded as a process to detect (and measure) the change of the mechanical state of an object during its motion (or quiet

state). In this respect, the first and the second law of Newton complement each in the description of the mechanical state of an object with respect to the presence or absence the of a force.

The key Newtonian *concepts of force* (momentum, and energy), allow then to resolve the problem of the main effect of the action of a force on a material system: i.e., to produce a change in the *space-time* configuration of the material system (as it possess a mass m). Therefore, regardless of the type of force acting on the system, (be it one of the four fundamental forces such as gravity, electrostatic, nuclear, or a more complex one) its effect is a modification of a *space-time “state”* and its intrinsically connected pattern under the exact description of mathematical form of the interaction between (point-like) particles. The force itself may depend on different parameters, like mass (i.e., for gravity force), charge (i.e., in electrostatic interaction), covalent bond strength or more complex parameters (and properties) of the investigated system. But the final result of its action is always a change in the measurable quantities of space, time, (and matter).

3. INTER-PARTICLES INTERACTION IN NANOSCIENCE: GENERALIZATION OF THE CONCEPT OF FORCE

The study of the inter-particles interaction represent a fundamental aspect in the investigation of the complex physics phenomena in many-body systems. Self-assembly of nanoparticles and nanostructures is a major field of research in current nanoscience, due to the unique properties of the generated materials. As inter-particle interactions play a crucial role in determining the morphology and architecture of materials assemblies, a comprehensive study of this topic, represent then a first important step for the understanding of the complex and cooperative behaviour in advanced functional materials [5-7].

In this respect, the physics teaching programs can be designed in a highly flexible and modern way, with the aim of going beyond the traditional curricula, which provide the study of a limited number of relatively simple forces (such as, gravitational, magnetic, electrostatic, elastic, friction force, and so on). Various strategies can be adopted to efficiently effort this point, within a physics-based approach.

The first step consists in the inclusion, into a new and more general conceptual framework, of the relevant forces encountered in the study of nanoscience and nanotechnology. As shown in Figure 1, it is possible to proceed with a generalization of the concept of interaction to the study of many-body systems. The new conceptual framework allows to integrate the study of the forces treated in traditional curriculum together with a number relevant complex interactions encountered in modern nanoscience. In this case the Newtonian space-time change of the (individual) particles is

framed within the more complex space-time evolution of the collective behaviour of a many-body systems [7, 8].

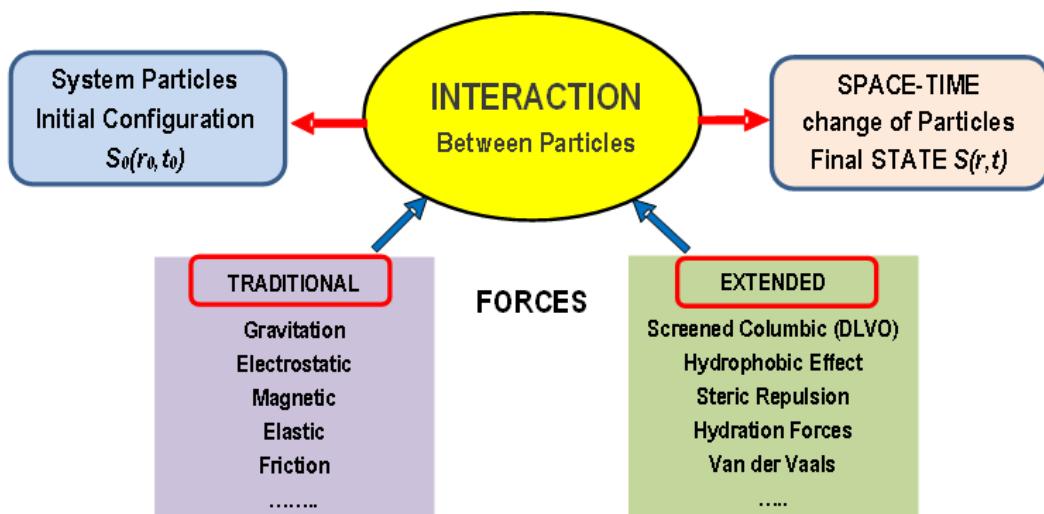


Figure 1. Conceptual framework for the study of the interaction within the many-body systems of modern nanoscience and nanotechnology.

4. INTERACTION AND SELF-ASSEMBLY IN NANOTECHNOLOGY: THE OBJECTIVES OF AN INTEGRATION CHALLENGE

Together with the concept of many-body interaction, the concept of self-assembly represent a central topic in nanoscience and nanotechnology. Self-assembly is the process in which a disordered system with many components turns into an orderly and stable structure with a minimum energy configuration. The use of self-assembly has been demonstrated to be one of the promising bottom-up methods for the design and construction of highly functional nanomaterials as well as a tool to test emerging properties of complex materials [6-11]. The combination of molecular interactions together with the ability to control both length scale and structural morphologies [12-17], makes nanomaterials particularly interesting for the development of transdisciplinary teaching programs at university.

From an educational point of view, particularly interesting is the study of traditional amphiphiles (and amphiphilic block copolymers), as those systems represent the precursor of the modern molecular building blocks in nanoscience. The possibility of molecular control by tuning the desired architecture (or polymer composition) makes these systems a versatile tool to study, in a convenient way, the rich and complex phenomenology in the field of nanoscience and nanotechnology, and stimulates the route

for the rational design and engineering of materials with desired properties [18-24].

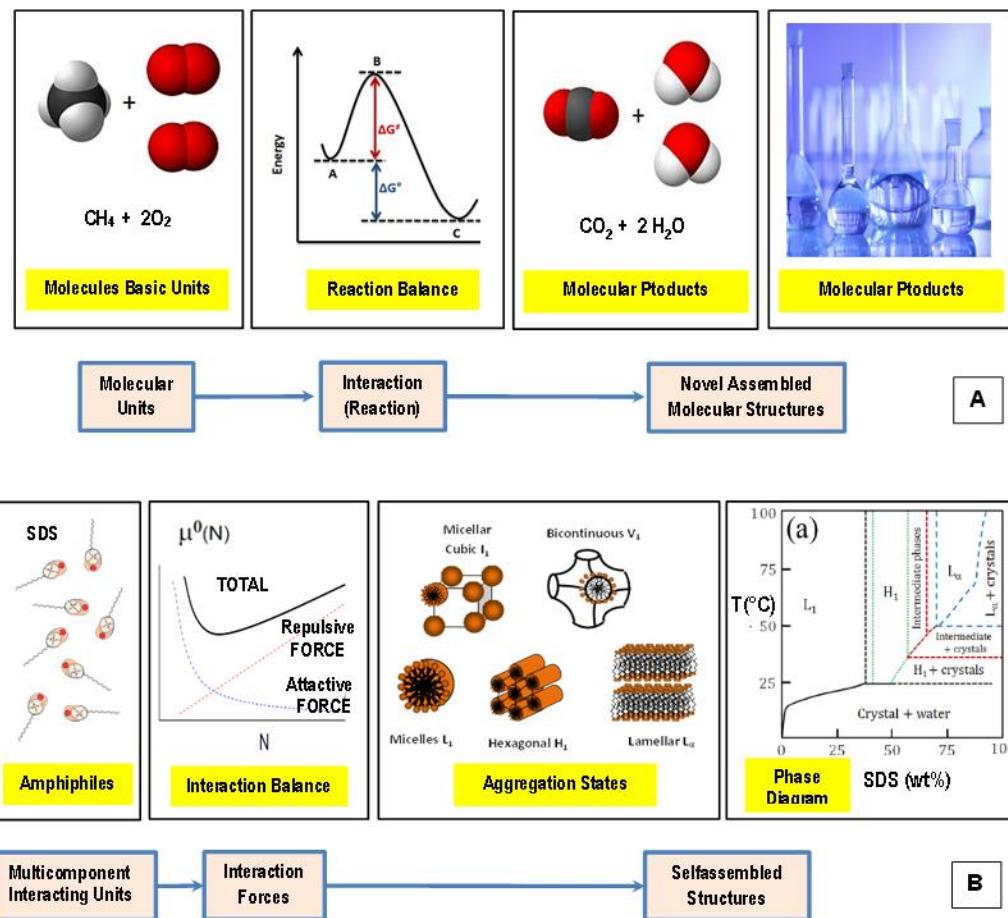


Figure 2. Example of two different selfassembly processes in multicomponent systems. The main features of a simple chemical reaction (A) shows strong similarity with the main characteristics of a selfassembly process involving a traditional amphiphile (sodium dodecyl sulphate - SDS).

From a didactic point of view it is possible to highlight the general aspect of the concept of self-assembly by making a similitude between a chemical reaction and the spontaneous formation of aggregates of amphiphilic molecules. At the same time it is important to point out the substantial differences, such as the reversibility/irreversibility of the two processes. Similarly to a chemical reaction, in fact, starting from an initial quantity of interacting basic units (initial compounds), we obtain a set of final products (aggregates), characterized by different morphologies that depends on the main system parameters (such as concentration and temperature).

In Figure 2 we compare the main steps of a chemical reaction (A) with the main features of the selfassembly process of a sodium dodecyl sulphate (SDS) amphiphile (B). Such an approach allow to introduce a new way of treating the complex variety of topics

within the nanoscience field. It also stimulates the discovery of important links between physics, chemistry, material science and engineering, thus highlighting the interdisciplinary aspects of the scientific knowledge.

5. SOFT INTERACTIONS IN NANOSCIENCE: BEYOND THE CONCEPT OF PAIRWISE INTERACTION BETWEEN POINT-LIKE PARTICLES

One of the the main characteristics of the selfassembly processes in nanoscience is the weakness of the involved forces (soft interactions) together to the involvement of a multiplicity of interaction site. These forces (due to their action on many-body systems) have some peculiar characteristics that distinguish them from the forces treated in traditional curricula. Despite the weakness of the interactions involved, the relevant number of these forces produce, in fact an overall effect which is strong enough to hold together different molecular structures (building blocks). Detailed treatment of the main soft (non-covalent) forces acting in nanostructures self-assembly (such as the hydrogen bonding, hydrophobic effects, screened electrostatic interaction, steric repulsion and van der Waals forces [25-27]) represents then an important and fundamental upgrade of modern approach in physics curriculum.

The involvement of a multiplicity of interaction sites, which is one of the main peculiar aspect of soft interactions, requires a substantial change in how these new topics must be addressed within a physics teaching program, with respect to the traditional Newtonian framework. We give a brief overview of some of the peculiar characteristic of the main soft interaction which play a prominent role in the many-body systems in the field of nanotechnology.

The *hydrogen-bonding (H-bonding)* is an highly directional, relatively strong, and specific interaction present in many organic molecules, and is responsible for supramolecular ordering in many biological systems [28-30]. The presence of hydrogen bonds (H-bond) makes nanostructured materials (such as biomolecules) substantially stronger upon forming a network (so called *H-bond cooperativity effect*) [31]. This circumstance is essential for many important functions in biological systems as H-bond are strong enough to bind biomolecules together but weak enough, when necessary, to be broken inside living organisms. H-bond interactions account for many biological processes such as the DNA base pairing, secondary and tertiary protein structure, carbohydrate hydration [32-34] as well as a range of unusual properties of water [35-37].

Together with the hydrogen bond, the *hydrophobic effect* is another important driving force of the nanomaterial self-assembly into various supramolecular structures [38]. The hydrophobic effect plays an important role in many soft matter systems as it regulates the tendency of nonpolar (hydrophobic) molecules to self-aggregate [38-43]. When non polar

molecules are dissolved in water, the disruption of the H-bonding water network favorites a rearrangement of the water molecules around the nonpolar molecules. This effect correspond to an effective mutual attraction (*hydrophobic interaction*) between the non-polar molecules, caused by the disruption of the H-bonding water network around the hydrophobe, followed by the rearrangement of new hydrogen bonds to form an ice-like cage structure (*clathrate*).

The hydrophobic effect plays a crucial role not only in the formation of amphiphilic micellar aggregates, but also for a wide range of other biological processes in protein, bio-membranes and biological systems [44-51]. For example, hydrophobic interactions are important in keeping a protein alive and biologically active through the folding processes which allow the protein to decrease its surface and reduce undesirable interactions with water [52-54].

The H-bond interaction and the hydrophobic effect represent important forces that, through their cooperative behavior, stabilize the nanostructures in their solution environment. There are three other important interactions that confer, through a spatially distributed action, a colloidal stability to the nanostructures in complex materials. These interaction are the *electrostatic stabilization* (or charge stabilization through an electrical double layer), *steric stabilization* (obtained with adsorbed or chemically attached polymeric macromolecules to the nanoparticles surface) and *depletion stabilization* (obtained by inserting free polymer in the dispersion medium) [55-57]. In the last two cases the presence of the polymer that occupies a certain amount of space generate an “effective repulsion” due to both volume restriction and interpenetration effects of polymeric molecules [55-59]. The degree of the stability is strongly dependent on the amount of excluded volume and on the sizes and geometries of the excluded particles.

6. MANY-BODY INTERACTION: SEARCHING APPROXIMATE SOLUTIONS FOR UNSOLVABLE PROBLEMS

A many-body system composed of multicomponent units interacting each other is impossible to solve exactly, except for very simple cases (such as in random field theory, 1D Ising model). However, the study of the behaviour of large and complex multicomponent system can be addressed by investigating simpler stochastic approximated model. Among them, one of the most widely used is represented by the *mean-field approximation (MFA)* [60], also known as *self-consistent field theory*. In a mean field approach the effect on any given individual elements of all the remaining component units, within a nay-body system, can be approximated by a single averaged effect. The n-body system is then replaced by a 1-body problem, through the suitable

choice of approximate external field that replaces the interaction of all the other particles to an arbitrary particle.

Another interesting approach for the solution of the problem of a many-body interacting system is given by solving the *Ornstein-Zernike (O.Z.) integral equation*, developed in the framework of liquid state theory [61, 62]. The integral equations approach has been employed to study the range and strength of a wide range of interparticle interactions in different systems of nanoscience including dendrimers, amphiphiles, proteins, and lipid bilayer vesicles [63-67]. A classical theoretical approach that make use of the O-Z approach to determine the nanoparticles interaction is given by the so called *D.L.V.O. theory* [56]. Within this approach the inter-particles interaction potential is determined by the balance between the Van der Waals (attractive) forces, and the screened Coulomb (repulsive) interaction. It is worth pointing that the application of the DLVO potential for the analysis of the interactions between nanoparticles evidenced the difficulty associated with having to rationalize the charge strength parameters in charged multi-components complex systems [68-71].

It is worth pointing that those approaches need a deep mathematical background preparation, as well as a proper analysis of the numerical solution methods. In this respect the teaching aspect should have its major emphasis on the methods that allow to approach the solution of specific many-body problems in the field of nanoscience. The lectures can be profitably organized as follows: various arguments of the program are first briefly introduced, and then specific problems are solved in full detail within the main aspects of the peculiar course of studies. In this case the main focus will be one's autonomy in the practice of specific theoretical approach, rather than in a systematic presentation of the well-established lessons covered by the course.

7. MOLECULAR DYNAMIC STEPWISE SOLUTION OF NEWTON'S LAW: PERSPECTIVE AND CRITICAL ISSUES

Molecular dynamic (MD) simulation try to circumvents the problem of the many-body interacting system by numerically integrating Newton's equations of motion, by means of an iterative computational approach [72, 73].

In multicomponent systems composed of many interacting particles, the forces between the particles are calculated using interatomic potentials or molecular force fields. In Figure 3 a schematic representation of the molecular dynamic approach is reported, together with the main approximated forces (force field) involved in multi-component system of nanoscience [72-73].

Once the system is built in its initial configuration (the cell), the forces acting on every atom are obtained through the solution of the force-fields equations, during small

integration time steps. In this case the potential energy is calculated starting from the initial molecular structure configuration. The form of the inter-particles interaction plays a crucial role in determining, with its mathematical expression, the numerical solution of the molecular dynamics simulation. This is a central point that allow a suitable solution to a problem that otherwise would have no solution.

The relative simplicity in the mathematical form of the force-field representation of the molecular interaction (such as springs for bond length and angles, periodic functions for bond rotations, Lennard–Jones potentials for van der Waals, and the Coulomb's law for the electrostatic interactions) [71-73] assures that the energy and forces calculations are extremely fast even for large systems (Figure 3).

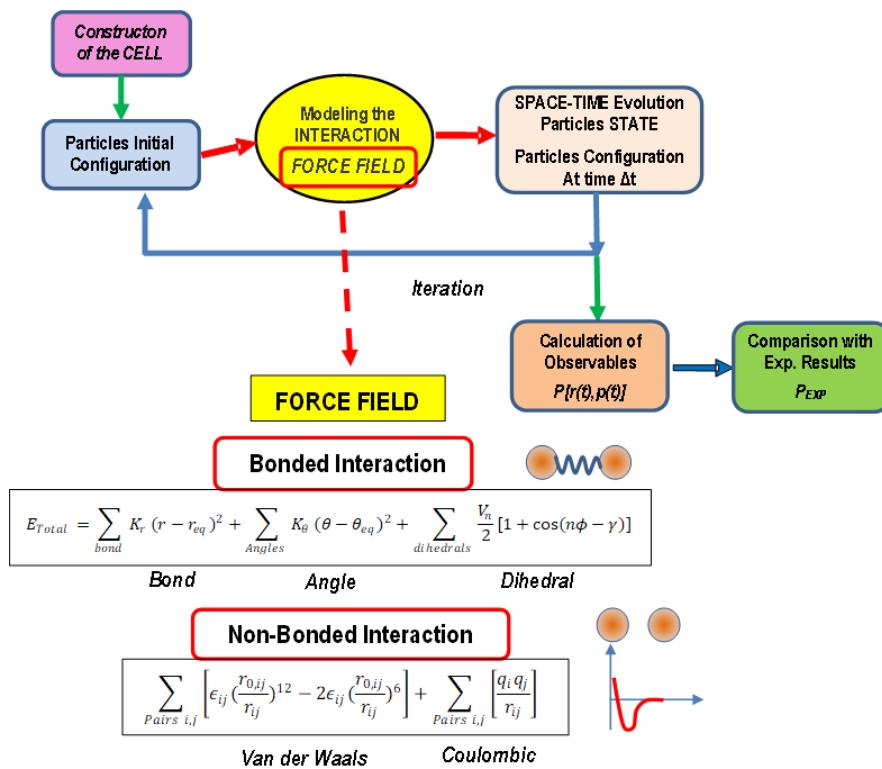


Figure 3. Schematic representation of the molecular dynamic approach and the main interactions (force fields) within a multi-component system of nanoscience.

The performances of simulations has been increased by recent methodological advances and high performance computing facility. Recently, an increasing number of molecular dynamics (MD) investigations have been partnered with experimental approaches [74-77], as computer simulations can track the system complex behaviour across a vast space-time scales ranges, otherwise inaccessible with traditional experiments. Novel MD computational methods have assumed in the last decades an ever growing importance in the field of nanoscience and nanotechnology. Computational

physics methods and molecular dynamic approaches, are expected to significantly increase the investigation capacity in physics of many-body systems. The increase of the educational aspects of this field of investigation benefits from the ease of finding on the web many of the resources necessary for learners. For those reasons, it is expected that this approach to nanoscience will impact the trajectory of the nanotechnology industry and academia. Finally. It is worth pointing that in some specific cases the practices of MD simulation do not achieve the precision needed to predict complex structural description in many multicomponent systems. In these cases the support from experimental approaches are necessary.

8. SUPRAMOLECULAR STRUCTURES AND FORCES: BEYOND THE CONCEPT OF PAIR-INTERACTION

In nanoscience the self-assembly processes between disordered basic units can form highly functional structures through a spontaneous organization of the basic units (building blocks). This level, that represent the most advanced stage in modern approaches for of nanoscience, is based on the concept of *supramolecular interaction* which is established between building blocks. Construction of advanced materials are obtained by employing suitable driving forces (*supramolecular forces*), including hydrogen bonding, host-guest recognition, electrostatic forces, metal coordination and π - π stacking interaction [78-85].

Interaction between Building Blocks and Supramolecular Structures

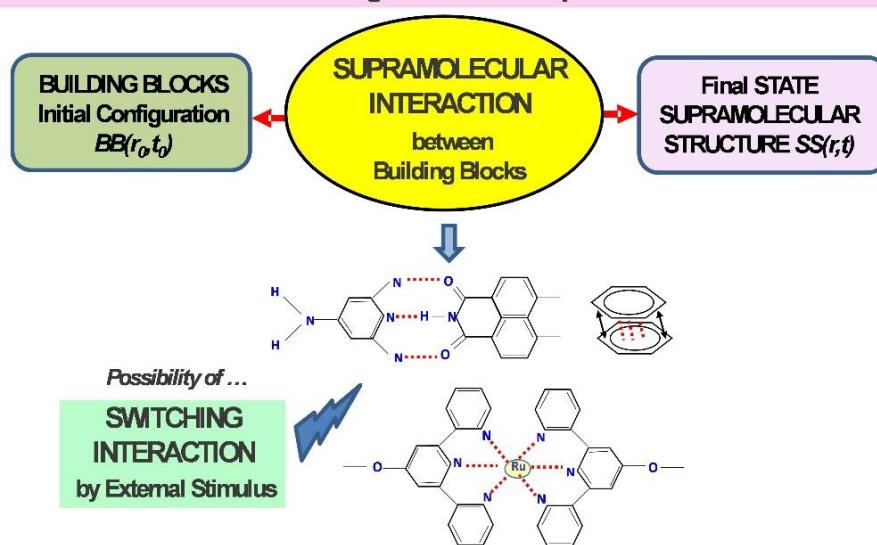


Figure 4. Conceptual framework for the study of supramolecular interactions in modern nanoscience and nanotechnology.

The combination of the dynamic (and sometimes reversible) nature of non-covalent interactions with the new topological features and multi-functionality of building blocks provides a versatile strategy for preparation of novel, advanced (nanostructured) functional materials [86-91].

This stage of the material evolution evidences how the reversible nature of the interactions may allow a dynamic switching of the generated nano-structures, with a modification of the morphology/function, in response to various external stimuli (such as pH, stress, temperature, electromagnetic radiation). For example the self-assembly nanostructures could disassemble upon the activation of an external stimulus such as ultraviolet (UV) electromagnetic radiation or pH, and this process can be exploited for potential applications in the field of controlled drug delivery.

The analysis of the innovative aspects of the study of the supramolecular interactions encountered in the field of nanoscience suggests to adopt, for interdisciplinary and educational purposes, a *conceptual scheme* based on the following three stages: (see Figure 4):

- *Building Blocks:* They are not only atoms and molecules, but span a wide range of nano- and mesoscopic structures, with different chemical compositions, shapes and functionalities. Examples include hybrid units containing crystals, colloids, lipid bi-layers, cyclodextrins, carbohydrates and peptides.
- *Supramolecular Interaction:* It usually involves combination of different soft interaction between interacting sites. The interacting forces often occur between different sites of the building blocks and may present some dynamic switching, that may activate a structural response of the system to various external stimuli.
- *Functional Supramolecular Structure:* The self-assembled nano-structure are expected to have a high function/performance suitable for advanced nanotechnology application.

As an example, the molecular recognition processes of a host–guest system consisting of a receptor molecule (host) interacting with a ligand molecule (guest) through noncovalent interactions can be inserted in the more general framework of the supramolecular interactions. The construction of supramolecular nanostructures based on host–guest interaction provides, in fact, a flexible platform for the development of a wide range of novel smart nanomaterials and functional supramolecular devices [92-95].

CONCLUSION

A key challenge for the efficient development of nanoscience and nanotechnology is based on the education and training of a new generation of skilled workers in the

multidisciplinary perspectives of the rapid progress stimulated by the new technologies. This require an update of the key concept usually taught within the science and technology curricula.

The concept of force and interaction in the many-body systems of modern nanotechnology presents a more complex characteristics than that encountered in basic principles of traditional physics programs. As multicomponent systems in nanoscience typically consist of a large number of interacting nanoparticles, it is impossible to determine, with high precision, the properties of such complex systems by solving analytically the corresponding set of equation of motion. Moreover most of the forces and interactions involved go beyond concept of pairwise interaction between point-like particles. This requires a deepening of these issues in order to provide an update of the key concepts based on current nanotechnology discoveries.

In this chapter, we present a review of the concept of force and its evolution within the framework of the recent discoveries in the field of nanotechnology. We also propose a conceptual framework for an upgrade of the concept of interaction within the modern approaches of academic physics programs.

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Chapter 6

A CONIC PENDULUM OF VARIABLE LENGTH ANALYSED BY WAVELETS

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ABSTRACT

Mathematics and Physics are disciplines interconnected for teaching purposes. Function and signal analysis play a key role in many scientific curricula. In particular, Wavelet Transform (WT) is increasingly applied to detect information on time dependent periodicities present in a signal. In this framework, in dealing with WT analysis within university courses it is often advantageous to adopt an integrated mathematical and physical approach. In this paper, we report the results obtained by the application of WT analysis to the motion of a very easy to realize system, i.e., a variable length conic pendulum. It is shown how WT allows to get information, in a straightforward way, on the time evolution of the registered signal frequency content.

Keywords: conic pendulum, Fourier analysis, wavelet analysis

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INTRODUCTION

Following Galileo Galilei, Mathematics is the alphabet with which God wrote the universe [1]. As a matter of fact, Mathematics is also the elective tool for theoretically modeling the Physics phenomena also for a comparison with experimental data.

In this framework, signal processing has a key role in different experimental fields, including Physics, Chemistry, Biology, Neutron scattering, Meteorology [2-10]. In particular Wavelet Transform (WT) is more and more widely employed in signal processing analysis for several, different purposes, such as multicsaling and trend analysis, revealing to be highly effective when it is essential to get information on the time evolution of the frequencies content of complex signals [11-16]. In fact, from an educational point of view, an important issue to be taken into account is that of updated programs. This leads to extract from a lot of contents, models and examples which are suitable for the interested student level, seeking a balance between two opposing tendencies. On one hand there is the need to simplify the educational material, depending on the student level of skills and abilities, to adapt the contents to the available time. On the other hand, there is the demand for programme updates due to the obsolescence of the contents, and therefore the need to consider recent research developments that are considered relevant. Furthermore, some of recent developments can be often unknown to some teachers which instead prefer stabilized topics, with definitive results acquired a long time ago. In other ways, it should be taken into account that many experimental and theoretical results, even if not too recent, can be in contrast with the contents usually proposed in standard university manuals, these latter being often uncritically repeated and therefore usually hard to question [17-19].

The present work furnishes an example of application of WT analysis to the specific case of the motion of a variable length conic pendulum. It will be shown that in this case, the WT approach is to be preferred to Fourier Transform since it is able to furnish information also on the time dependence of the signal frequencies content.

FOURIER AND WAVELET TRANSFORMS

One of the most powerful tool commonly employed for the analysis of signals, is the Fourier analysis; this technique, developed by J. Fourier, in the first twenty years of 1800, allows to study a signal in the frequency domain starting from the time domain [20]. However, the Fourier Transform (FT), besides treating efficiently only linear problems, hides information about time. Efforts to overcome these limits led D. Gabor, in 1946, to the definition of the Short Time Fourier Transform (STFT); this latter approach allows, through the multiplication of the signal with a “window” function, to consider it linear

within a window range, thus permitting also the analysis of non-linear signals, and to obtain a representation of the signal both in frequency and in time [21]. However this type of analysis suffers from a limit: once the “window” is chosen it is kept fixed for the whole course of the analysis so precluding the possibility of modifications; moreover, due to the Uncertainty Principle, a higher time resolution decreases the frequency one, and vice versa.

The Wavelet Transform (WT) analysis was formulated in response to these limits; from the early 1900s up until the 1970s, there were different approaches to this topic: on one hand, the mathematical community tried to overcome the analytical limits of the STFT starting to conceive a more customizable approach; on the other hand, from an experimental point of view, different algorithms, closely connected with WT analysis, were suggested both for signal and image analysis. These approaches to WT analysis started in 1909 with the work of the German mathematician A. Haar [22], who investigated the corresponding orthonormal bases, and continued with several and different contributions. Starting from that of the physicist K. Wilson [23] and of several French researchers working in the field of digital signals, i.e., A. Croisier, D. Esteban, C. Galand [24], continuing with that of D. Marr [25] in the treatment of the human vision system, until to 1975, date which can be taken as indicative of the birth of the analysis wavelet. In this year, J. Morlet, differently from STFT where the width of Gabor's “window” function was kept fixed while filling it with oscillations of different frequency, blocked the number of oscillations in the function changing its amplitude through compressions and extensions. The Morlet's work [26] was continued by Y. Meyer [27], physician of Marseilles, and by A. Grossman [28], professor of the Ecole Polytechnique. Then S. Mallat, starting from 1986, formalized the wavelet theory, delineating the extension to the discrete case. In this context he enunciates the “Theory of multiresolution analysis”, capable to transfer the discrete wavelet transform theory to all those algorithms, such as the Pyramid Algorithm, used in image analysis although never formalized in the context of WT analysis. Starting from the work of Mallat [29] and I. Daubechies [30], around 1987, built the orthonormal wavelet bases, which became a milestone for WT applications.

From a mathematical point of view, the Fourier series allows to express a periodic function $y(t + T) = y(t)$, with period $T = \frac{2\pi}{\omega}$, ω being a frequency, as [31-32]:

$$y(t) = \sum_{n=0}^{\infty} [C_n \cos(n\omega t) + S_n \sin(n\omega t)] \quad (1)$$

C_n and S_n being the Fourier coefficients.

The Fourier transform is an extension of the Fourier series for non-periodic functions:

$$\hat{Y}(v) = \int_{-\infty}^{+\infty} y(t) e^{-i2\pi v t} dt \quad (2)$$

WT associates to $y(t)$, a function of the two variables m , τ , $W(m, \tau)$, where the parameter $m > 0$ denotes the scale and its value is the inverse of the frequency while the parameter τ indicates a shift of time along the time axis. WT decomposes $y(t)$ into a set of wavelets components $\frac{1}{\sqrt{m}} \psi\left(\frac{t-\tau}{m}\right)$, that can be chosen according to the similarity degree with $y(t)$, as it follows:

$$W(m, \tau) = \frac{1}{\sqrt{m}} \int_{-\infty}^{+\infty} y(t) \psi^*\left(\frac{t-\tau}{m}\right) dt \quad (3)$$

where ψ^* denotes the conjugate complex of the function ψ .

Differently from FT, which shows only which signal frequencies are present, WT also shows where, or at what scale, they are [33-48].

THE CONIC PENDULUM

A conic pendulum is made of a mass, hanged by an inextensible string having negligible mass. The mass, that is under the action of gravity, moves with an initial tangential velocity. When the frictions connected to both the suspension constraint and viscosity of the medium in which the pendulum is immersed are negligible, the mass performs a rotary motion on an ideal horizontal plan with a linear velocity that is constant in modulus. Under these ideal conditions, where no energy dissipation occurs, if the pendulum length is constant in time, the mass rotates following a circular trajectory while the mass-string system describes a conic surface remaining in a state of dynamical equilibrium. The corresponding time law projected along an arbitrary vertical plane is a sinusoidal function characterized by a constant angular velocity whose Fourier transform furnishes a peak centred at the motion angular frequency [49-51].

This work describes an experiment where the length of the conic pendulum string decreases as a function of time and, consequently, the frequency of the motion increases giving rise to a chirp-like behaviour for the motion time law. In particular, in this case, to follow the evolution of the time of the pendulum frequency, a wavelet approach is applied.

More in details, at first different period values of the pendulum are determined with fixed lengths, and then the motion time law is registered while the string length diminishes as a function of time.

The experimental set-up includes:

- A 3 m long string;
- oscillating mass whose weight is 75,14 g
- a fixed support to fix the pendulum;
- a step by step rotating device for changing the pendulum length;
- a computer equipped with video data acquisition program and Matlab-Simulink software, i.e., Image Processing Toolbox and the Computer Vision Toolbox;
- The system length variation as a function of time was assured by the step by step rotating device and was registered through a PC.

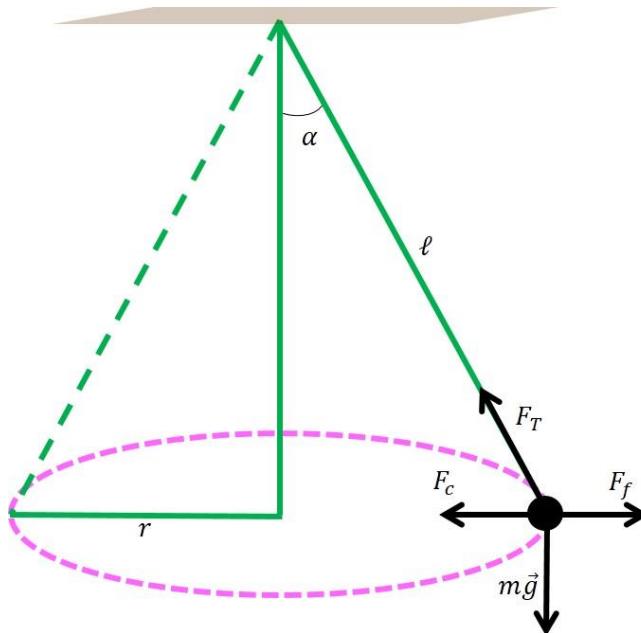


Figure 1. Force decomposition for a conic pendulum.

The case of variable length is taken into account with the purpose to determine how the rotational period of the pendulum varies as a function of the string length. In Figure 1 the force decomposition for a conic pendulum is reported.

THEORETICAL BACKGROUND AND EXPERIENCE PROCEDURE

When the length of the string does not vary, it is possible to describe the motion along the x and y axes of the pendulum [52-55].

For the y axis, one has:

$$F_T \cdot \cos\alpha = mg \quad (4)$$

and for the x axis, one has:

$$F_T \cdot \sin\alpha = m \frac{v^2}{r} \quad (5)$$

Since $r = \ell \cdot \sin\alpha \rightarrow \sin\alpha = \frac{r}{\ell}$, one has for the x-axis component:

$$F_T = \frac{m \cdot v^2}{r \cdot \sin\alpha} = \frac{m \cdot v^2}{r} \cdot \frac{\ell}{r} = \frac{m \cdot v^2 \ell}{r^2} \quad (6)$$

and being $v = \omega \cdot r \rightarrow v^2 = \omega^2 \cdot r^2$ it is $\cos\alpha = \frac{g}{\ell \cdot \omega^2}$ and hence:

$$\omega = \sqrt{\frac{g}{\ell \cdot \cos\alpha}} \quad (7)$$

Therefore, under these conditions, the rotating period results:

$$T = \frac{2\pi}{\omega} \rightarrow T = 2\pi \cdot \sqrt{\frac{\ell \cdot \cos\alpha}{g}} \quad (8)$$

Let us now take into account the case of variable length; the purpose here is to determine how the rotational period of the pendulum varies as a function of the length of the string.

Introducing the quantity $s(t)$ for the linear displacement of the pendulum for an angular rotation $\theta(t)$ on a plane orthogonal to the y axis:

$$s(t) = r(t) \cdot \theta(t) = \ell(t) \sin\alpha(t) \cdot \theta(t) \quad (9)$$

Now, assuming that:

- i. the variation rate of the pendulum length, i.e., $\frac{d\ell}{dt}$, is constant, so that $\frac{d^2\ell}{dt^2}$ is equal to 0;
- ii. $\frac{d\ell}{dt}$ and $\frac{d\alpha}{dt}$ are small in respect to $\frac{d\theta}{dt}$, i.e., the rotational velocity of pendulum on the plane orthogonal to y axis.

One can express the corresponding time law projected along an arbitrary vertical plane as a sinusoidal function characterized by a variable angular velocity:

$$S(t) = \frac{s(t)}{A(t)} = \operatorname{sen}(\omega t + \varphi) \quad (10)$$

where $A(t)$ represents the amplitude of motion, $\omega t + \phi$ the phase of motion, φ the initial phase and is:

$$\omega = \omega_0 + \gamma t \quad (11)$$

where ω_0 is the initial pulsation and $\gamma = \frac{d^2\theta}{dt^2}$ is the angular acceleration.

The experiment was performed in three different sections during which the period was evaluated by a simple calculation, by taking into account different stationary oscillation and, finally, in a dynamic way by decreasing the pendulum length. In all the three cases, a force F was applied, tangentially with respect to the circumference, to a mass of 75,19g.

In particular, in the first experiment phase, once the radius of the circumferences described by the pendulum was established, the tangent of the angle between the static pendulum equilibrium position and the dynamic equilibrium trajectory can be evaluated; from the tangent it is then possible to extract the angle cosine which allows to determine the period, $T = 2\pi \cdot \sqrt{\frac{\ell \cdot \cos\alpha}{g}}$.

Concerning the stationary case, the experiment was performed by measuring the period by means of chronometers, taking into account several oscillations in order to get an accuracy more precise. Table 1 shows the values registered during the two cases.

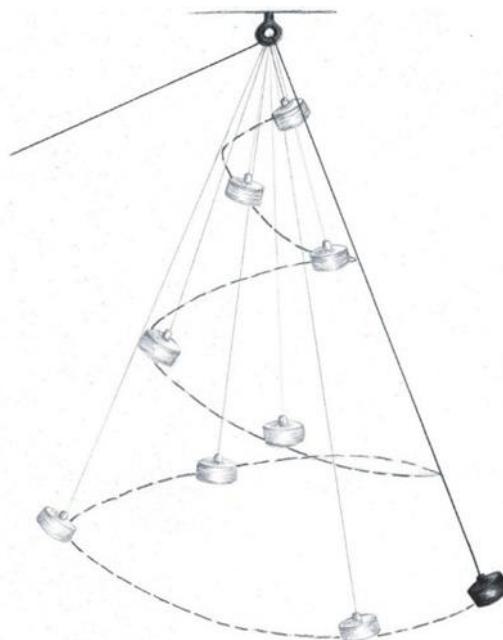


Figure 2. A simple sketch of a variable length conic pendulum.

Table 1. Pendulum length ℓ , radius R , $\tan\alpha$, $\cos\alpha$, period T evaluated by a simple calculation ($T_{evaluated}(s)$) and period evaluated by taking into account different stationary oscillation ($T_{experimental}(s)$) for three different measurements of pendulum length

ℓ (m) \pm 0,001	R(m) \pm 0,001	$\tan\alpha$	$\cos\alpha$	$T_{evaluated}$ (s)	$T_{experimental}$ (s) \pm 0,01
2,875	0,415	0,144	0,990	3,390	3,410
	0,495	0,172	0,985	3,380	3,450
	0,497	0,173	0,986	3,380	3,450
2,775	0,493	0,178	0,985	3,320	3,370
	0,503	0,181	0,984	3,318	3,380
	0,509	0,183	0,984	3,318	3,350
2,575	0,533	0,207	0,979	3,188	3,210
	0,524	0,203	0,980	3,899	3,230
	0,503	0,195	0,981	3,191	3,150
2,375	0,475	0,200	0,981	3,065	3,180
	0,500	0,210	0,979	3,062	3,080
	0,440	0,185	0,983	3,068	3,020
2,175	0,475	0,218	0,977	2,927	2,960
	0,485	0,223	0,976	0,926	3,030
	0,435	0,200	0,981	0,934	2,890
1,975	0,415	0,210	0,979	2,793	2,760
	0,425	0,215	0,978	2,792	2,780
	0,445	0,205	0,980	2,794	2,840
1,775	0,405	0,226	0,975	2,643	2,720
	0,380	0,214	0,978	2,645	2,670
	0,370	0,208	0,979	2,648	2,770
1,375	0,400	0,290	0,960	2,309	2,720
	0,375	0,273	0,965	2,315	2,310
	0,475	0,345	0,945	2,291	2,410
0,975	0,340	0,349	0,944	1,929	2,030
	0,295	0,303	0,957	1,943	20,10
	0,150	0,154	0,988	1,974	1,970
0,875	0,265	0,303	0,957	1,84	1,870
	0,275	0,314	0,954	1,838	1,950
	0,250	0,286	0,961	1,845	1,960
0,775	0,280	0,361	0,941	1,719	1,850
	0,255	0,329	0,950	1,727	1,760
	0,265	0,342	0,916	1,723	1,770
0,675	0,160	0,237	0,973	1,632	1,830
	0,750	0,111	0,994	1,65	1,820
	0,125	0,185	0,848	1,523	1,810
0,575	0,125	0,217	0,977	1,51	1,620
	0,120	0,209	0,978	1,511	1,650
	0,170	0,296	0,956	1,494	1,690

As shown in the table, three different measurements were performed, one for each length of the string. By using the data in the table, it is possible to make a comparison between the two approaches. The data obtained using the stationary approach are reported in Figure 3.

Finally, in the third dynamic case, the pendulum length decreased following the equation:

$$\ell = \ell_0 + v_m \cdot (t_2 - t_1) \quad (12)$$

the velocity for the decreasing string length was $v_m = 0,1617 \pm 0,0001$

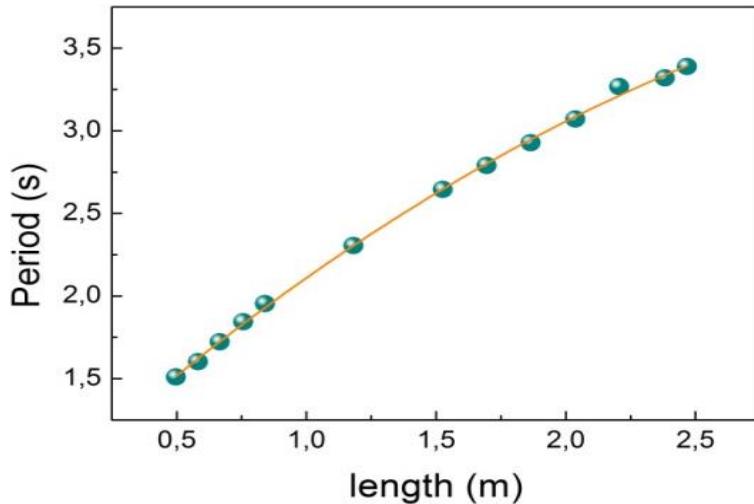


Figure 3. Data obtained using the stationary approach.

Table 2. Motion parameters, i.e., time, pendulum length and period, obtained by using an initial radius value of $r = 0,2\text{ m}$

t (s)	ℓ (m)	T (s)
$7,74 \pm 0,01$	$2,240 \pm 0,001$	$3,18 \pm 0,01$
$10,60 \pm 0,01$	$1,772 \pm 0,001$	$2,93 \pm 0,01$
$13,22 \pm 0,01$	$1,352 \pm 0,001$	$2,55 \pm 0,01$
$15,60 \pm 0,01$	$0,971 \pm 0,001$	$2,08 \pm 0,01$
$17,09 \pm 0,01$	$0,723 \pm 0,001$	$1,79 \pm 0,01$
$18,66 \pm 0,01$	$0,472 \pm 0,001$	$1,57 \pm 0,01$

Figure 4 shows the time dependence of the pendulum length varying from 2,240 m to 0,472 m.

The motion parameters were collected using an initial radius value of $r = 0,2\text{ m}$, through two different methodologies. In particular, the period values were registered at different times, as reported in Table 2.

Figure 5 shows the behaviour of angular pulsation as a function of time.

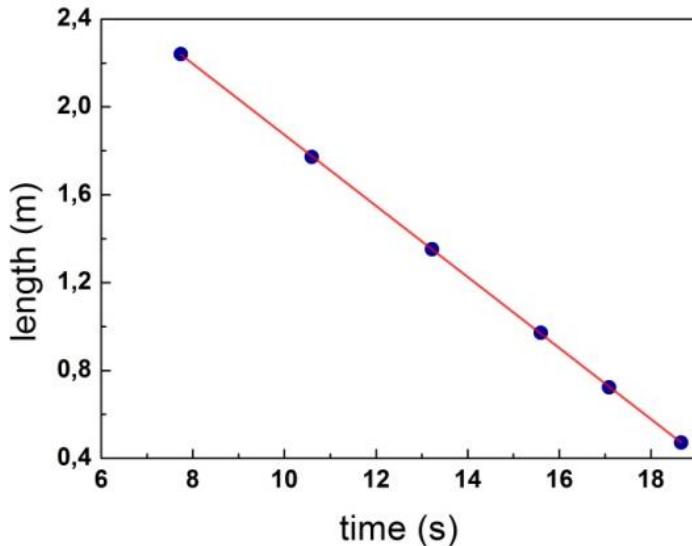


Figure 4. Time dependence of the pendulum length varying from 2,240 m to 0,472 m. In particular, $\ell = \ell_0 + v_m \cdot (t_2 - t_1)$, with $v_m = 0,1617 \pm 0,0001$.

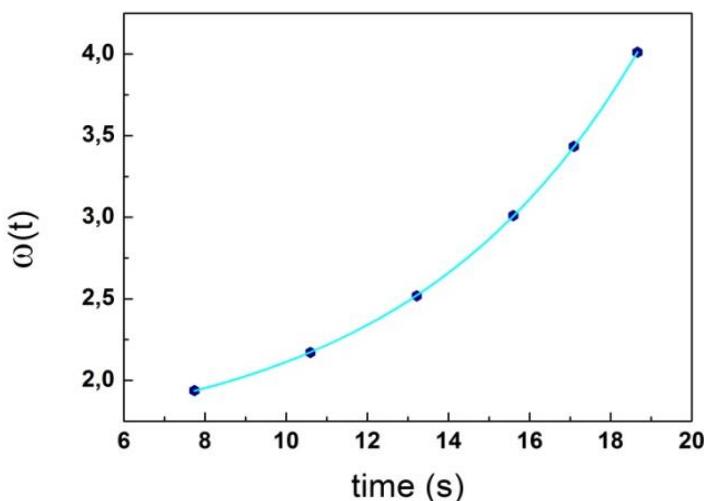


Figure 5. Time dependence of the pendulum pulsation.

The motion was registered by means of the video data acquisition program (with a Matlab-Simulink software, i.e., Image Processing Toolbox and the computer Vision Toolbox) put at the bottom of the suspended pendulum.

In Figure 6 the registered signal together with its FT and WT spectra are reported. More specifically, on the top of the figure the collected frequency dependent oscillation signal, under the condition of varying length; on the right of the figure its FT showing only an average of the registered signal frequencies; on the bottom of the figure the WT scalogram that shows how the oscillation pseudo-frequency changes with time [56-57].

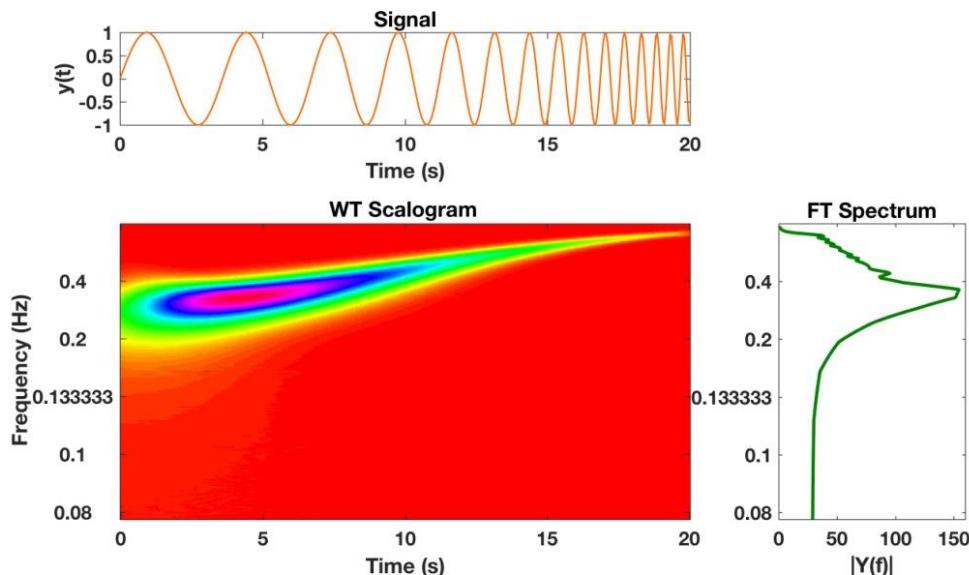


Figure 6. A comparison of the registered signal analysed by means of FT and WT. On the top of the figure the collected frequency dependent oscillation signal, under the condition of varying length; on the right of the figure its FT showing only an average of the registered signal frequencies; on the bottom of the figure the WT scalogram that shows how the oscillation pseudo-frequency changes with time.

CONCLUSION

Signal processing plays a key role in different experimental fields, including Physics, Chemistry, Biology, Neutron scattering and Meteorology. In this framework WT is widely employed for multiscaling and trend analysis allowing to get information on the time evolution of the frequencies content of signals. Nowadays, from the educational point of view, an important issue is to update programs looking both for a simplification of the educational material, depending on the student level of skills and abilities and for recent research developments which are considered relevant. In the present work a conic pendulum where its length decreases as a function of time is dealt. It is shown that the frequency of the rotatory motion increases giving rise to a chirp-like behaviour for the motion time law. In this case, to follow the evolution of the time of the pendulum frequency, a wavelet approach is applied. More specifically, a comparison between FT and WT is performed. The two approaches put into evidence the effects of the pendulum length change on the oscillation frequency. It clearly emerges that WT provides a straightforward simultaneous time-frequency analysis.

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Chapter 7

A NEW APPROACH TO THE ADIABATIC PISTON PROBLEM THROUGH THE ARDUINO BOARD AND INNOVATIVE FREQUENCY ANALYSIS PROCEDURES

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ABSTRACT

The adiabatic piston problem is the subject of great attention for the involved education aspects in advanced thermodynamics curricula. The aim of this work, which for the theoretical section is mainly based on the work published in 1996 by Crosignani B. and Di Porto P., is to examine the adiabatic piston time evolution towards the mechanical equilibrium (final pressure determination) and towards the thermal equilibrium (final temperature determination). In particular, it will be shown how, by means of a thermodynamics analysis is not possible to univocally determine the final state of the system; it will be shown how this indeterminacy can be overcome by using an appropriate kinetic model. In particular, the motion equations derived from a kinetic model allow to define the final equilibrium state once that the initial value of the piston position and the initial temperatures of the two component subsystems are defined. In this framework it will be shown how it is possible to evaluate the phase relations between the temperatures and the piston displacement by applying the Wavelet Cross Correlation approach. Finally the gas specific heat ratio is experimentally evaluated by measuring the oscillation period of an adiabatic piston, where the relevant physical parameters are

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collected through sensors connected to an Arduino board, by applying a Fourier transform approach.

Keywords: adiabatic piston, Wavelet Cross Correlation, gas specific heat ratio, Arduino board, Fourier transform

INTRODUCTION: THE ADIABATIC PISTON

The adiabatic piston [1-4] we are going to deal with consists of an adiabatic cylinder separated by an adiabatic septum, which determines two subsystems, A and B, each containing the same number of moles n of a perfect gas, as shown in Figure 1.

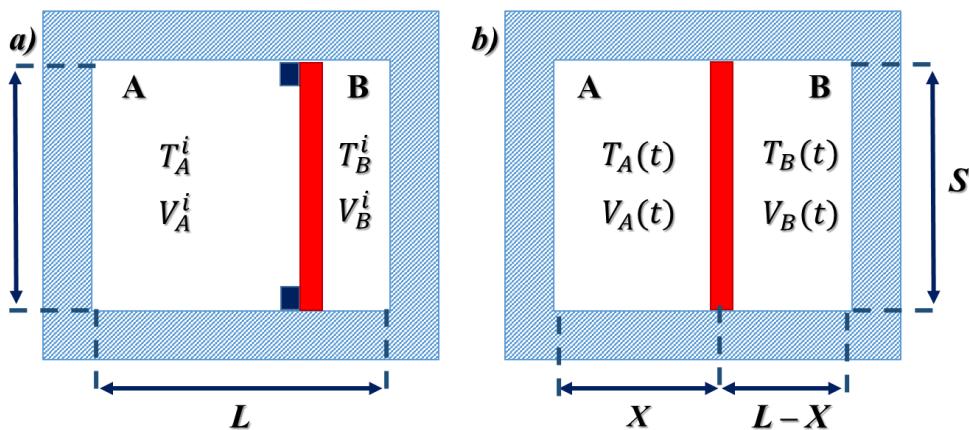


Figure 1. Sketch of the adiabatic piston taken into account in the present work; a) adiabatic piston configuration at time $t = 0$ when the equilibrium state is maintained by the use of physical constraints; b) adiabatic piston at the generic time t when the physical constraint is removed.

In the Figure S and L are the transverse area and the length of the cylinder, respectively.

Initially, at $t = 0$, the two subsystems A and B are in a state of constrained equilibrium; here the state of the two gases is defined by the values of the initial temperatures and volumes denoted in the following T_A^i , T_B^i , V_A^i , V_B^i , respectively. The initial pressure values of the two subsystems are known and are P_A^i and P_B^i with P_A^i different from P_B^i . Then, at $t > 0$ the constraint is removed.

The first part of this work moves from the nice paper published in 1996 by Crosignani B. and Di Porto P. [4] in which the approach to thermal equilibrium is dealt.

The first principle of thermodynamics furnishes a quantitative expression of the principle of energy conservation. For a system that can exchange energy only by means of heat and pressure work, for an infinitesimal exchanges, it can be expressed formally as follows:

$$dU = \delta Q - \delta L \quad (1)$$

where Q is heat and L is work.

In the case of an infinitesimal adiabatic transformation, $\delta Q = 0$, one has:

$$dU = -\delta L \quad (2)$$

Equation 2 shows that adiabatic work is independent on the path.

With reference to equation 1, it should be noted that the differential symbols for Q and L are denoted by δ . There is a fundamental difference between a property like the U on one side and the quantities Q and L on the other sides. A property like U always has a value that depends only on the state of the system. A transformation that causes a change in the state of the system causes a change in internal energy. Hence dU represents an infinitesimal variation of U . Q and L are not property of the system and depend on the path of transformation. Therefore δ is used to indicate infinitesimal quantity.

From a general point of view, one can assume that the internal energy U for our closed system is a function of T and V , i.e.,:

$$U = U(T, V) \quad (3)$$

Therefore it is possible to write:

$$dU = \left(\frac{\partial U}{\partial T}\right)_V dT + \left(\frac{\partial U}{\partial V}\right)_T dV \quad (4)$$

The thermal capacity at constant volume C_V represents the amount of heat to increase the temperature of dT when the system maintains constant volume:

$$C_V = \frac{1}{n} \left(\frac{\partial Q}{\partial T}\right)_V \quad (5)$$

where n is a number of moles of gas.

For a reversible transformation at constant volume one has $dU = \delta Q$, since there can be no work exchanges. The eqn. 5 can be rewritten:

$$C_V = \frac{1}{n} \left(\frac{\partial U}{\partial T}\right)_V \quad (6)$$

and substituting eqn. 6 in eqn. 4, one has:

$$dU = nC_V dT + \left(\frac{\partial U}{\partial V}\right)_T dV \quad (7)$$

For the application of this equation, the values of the derivative $\left(\frac{\partial U}{\partial V}\right)_T$ are required, values that in general must be determined experimentally. In the specific case in which the system under investigation is a perfect gas it is required that for all temperatures and pressures is:

$$PV = nRT ; \left(\frac{\partial U}{\partial V}\right)_T = 0 \quad (8)$$

Then, eqn. 7, for a perfect gas, becomes:

$$dU = nC_V dT \quad (9)$$

Eqn. 9 is always valid for a perfect gas, regardless of the type of transformation that is considered.

Taking into account the first principle of thermodynamics and that the variation of the perfect gas internal energy for each subsystem depends only on temperature, it is possible to obtain the following equality for the system taken into consideration:

$$T_A^i + T_B^i = T_A^f + T_B^f \quad (10)$$

Since at equilibrium the final pressures of the two systems A and B are the same, it is:

$$P_A^f = P_B^f \quad (11)$$

From the perfect gases state equation, $PV = nRT$, we have that:

$$P_A^f = \frac{nRT_A^f}{V_A^f} ; P_B^f = \frac{nRT_B^f}{V_B^f} \quad (12)$$

Therefore, the equality of the pressures in eqn. 11 reduces to:

$$\frac{T_A^f}{V_A^f} = \frac{T_B^f}{V_B^f} \quad (13)$$

being T_A^f , T_B^f , V_A^f , V_B^f the final temperatures and volumes, respectively. Using eqn. 13 and the equation of state one gets the following expression for the final pressure:

$$P^f = n \frac{RT_1^f}{V_1^f} \quad (14)$$

By multiplying the numerator and denominator of eqn. 6 for the quantity $(1 + T_B^f/T_A^f) = (1 + V_B^f/V_A^f)$, one has:

$$P^f = nR \frac{T_A^f(1+T_B^f/T_A^f)}{V_A^f(1+V_B^f/V_A^f)} = nR \frac{T_A^f+T_B^f}{V_A^f+V_B^f} = nR \frac{T_A^i+T_B^i}{V_A^i+V_B^i} \quad (15)$$

where, we have considered: $T_A^f + T_B^f = T_A^i + T_B^i$ and $V_A^f + V_B^f = V_A^i + V_B^i$.

As shown by eqn. 15, the equilibrium pressure can be predicted univocally, being it dependent only on the initial state of the two subsystems. The final temperatures T_A^f , T_B^f and volumes V_A^f , V_B^f can not be predicted, since they depend upon parameters lying outside the domain of the thermodynamics description.

From a general point of view, the determination of the final equilibrium state of the system can be considered as the search for the maximum of a particular state function that describes the system. In the thermodynamic case, for example, this role is absolved by the entropy and the parameters of the equilibrium are none other than the variables of the system that make this function maximum. This is analogous to the equilibrium conditions of a mechanical system whereby a minimum of potential energy must be determined. However, the dynamics laws do not always allow to unambiguously determine the system equilibrium position. For instance, in the mechanical system reported in Figure 2 (a), the principle of minimum provides $x = y = 0$. For the mechanical system in Figure 2 b), the same principle furnishes only the partial solution $y = 0$ while the x variable is not determined. However it should be stressed that the equilibrium position can be determined by solving the equations of motion.

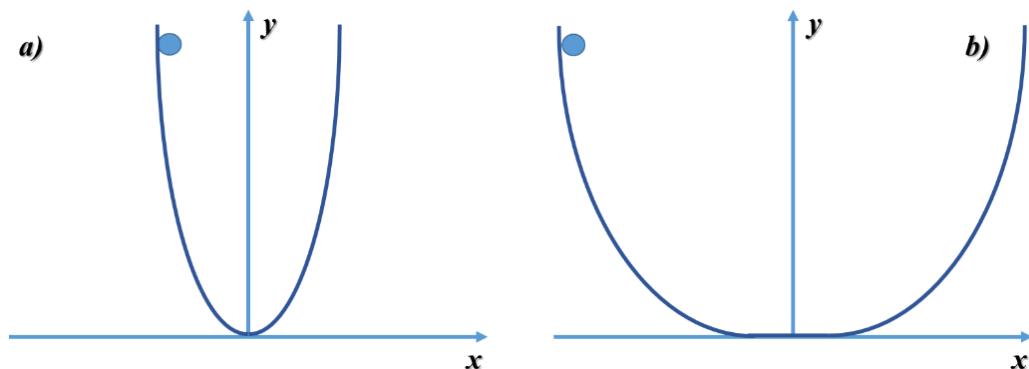


Figure 2. Ball rolling under the action of viscous friction forces. a) The minimum principle indicates the solution $x = y = 0$; b) the minimum principle only indicates the condition $y = 0$.

REVERSIBLE ADIABATIC TRANSFORMATIONS

In summary, the thermodynamics analysis [1] of the equilibrium states does not allow the determination of the final temperatures and volumes T_A^f , T_B^f , V_A^f , V_B^f of the two subsystems A and B.

Making reference to the system shown in Figure 1, the two subsystems A and B, each containing n moles of perfect gas, have a generic internal energy $U = nC_V T$; furthermore they have the following average quadratic velocity (v_m^2) along the X direction:

$$v_m^2 = \frac{k_B T}{m} \quad (16)$$

where k_B is the Boltzmann constant, T is the temperature and m is the mass of the gas particles.

To determine an equation of motion for the piston it is necessary to require that the temperatures T_A and T_B of the two subsystems A and B (and therefore the position of the piston) be defined at each instant of time t during a quasi-static transformation.

For the system under consideration [3], the total energy of the system is:

$$E = U_A + U_B + E_k \quad (17)$$

where U_A and U_B are the internal energies of the two systems and E_k is the kinetic energy of the piston.

Recalling that the internal energy is related to temperature (eqn. 9), it is possible to rewrite eqn. 17 as follows:

$$E = nC_V T_A + nC_V T_B + \frac{1}{2} M \dot{X}^2 \quad (18)$$

where M and \dot{X} are the mass and the velocity of the piston, respectively.

For the two subsystems A and B, the conditions defined for the perfect gas furnish:

$$P_A V_A = nRT_A ; P_B V_B = nRT_B \quad (19)$$

Deriving eqn. 18 with respect to time, one has:

$$\frac{dE}{dt} = \frac{nC_V dT_A}{dt} + \frac{nC_V dT_B}{dt} + M v \dot{v} \quad (20)$$

For the first principle of thermodynamics, one has:

$$nC_VdT_A = -P_AdV_A; nC_VdT_B = -P_BdV_B \quad (21)$$

Inserting eqn. 21 in eqn. 20 and taking into account the relations 19, one obtains for the piston motion:

$$M\ddot{v} = \frac{nRT_A}{X} - \frac{nRT_B}{L-X} \quad (22)$$

Using the perfect gas state eqn. 19, eqns. 21, and performing the derivative with respect to time, one gets:

$$\frac{nC_VdT_A}{dt} = -\frac{nRT_A}{X} \frac{dX}{dt} \quad (23)$$

$$\frac{nC_VdT_B}{dt} = \frac{nRT_B}{L-X} \frac{dX}{dt} \quad (24)$$

By integrating eqns. 23 and 24, one has:

$$T_AX^{\gamma-1} = const, T_B(L-X)^{\gamma-1} = const \quad (25)$$

where L is the total cylinder length $\gamma = c_P/c_V$ is the relationship between specific heat at constant pressure and volume.

Eqn. 25 refer to reversible adiabatic transformations. These transformations are responsible of the oscillation motion of the piston in which the force to which it is subjected is proportional to the difference of the pressures in the two subsystems.

It is useful to rewrite eqns. 23, 24 and 22 in a dimensionless form, i.e.,:

$$\dot{\Theta}_A = -(\gamma - 1)\Theta_A \frac{\Psi}{\Psi} \quad (26)$$

$$\dot{\Theta}_B = (\gamma - 1)\Theta_B \frac{\Psi}{1-\Psi} \quad (27)$$

$$\dot{\Psi} = \frac{\Theta_A}{\Psi} - \frac{\Theta_B}{1-\Psi} \quad (28)$$

where $\Theta_A = \frac{T_A}{T_\alpha}$, $\Theta_B = \frac{T_B}{T_\alpha}$, $T_\alpha = T_A + T_B$, $\Psi = \frac{X}{L}$, $\tau = \frac{t}{t_\alpha}$, $t_\alpha = \left(\frac{ML^2}{nRT_\alpha} \right)$ in which the time derivative is with respect to τ .

KINETIC MODEL FOR THE DETERMINATION OF EQUILIBRIUM

The solution found in eqn. 28 leaves the problem non-determinate since the piston will oscillate never reaching a final equilibrium state. This result derives from having not considered the finite velocity of the piston v_{piston} :

$$v_{piston} = \frac{dx}{dt} \quad (29)$$

in the variation of the momentum of the gas molecules due to the impacts against the piston walls [3-9].

Let us assume that, a generic molecule of the gas contained in the adiabatic piston, with velocity v_x along the x axis of the cylinder, impacts the wall after a displacement $x = v_x \Delta t$. For a fixed piston, the number of collisions of the gas molecules having a velocity between v_x and $v_x + dv_x$ will be:

$$\frac{N}{Sx} S v_x \Delta t f(v_x) dv_x \quad (30)$$

where S is the piston section, N is the Avogadro's number and:

$$f(v_x) = \left(\frac{m}{2\pi k_B T} \right)^{1/2} e^{-\frac{mv_x^2}{2\pi k_B T}} \quad (31)$$

which represents the Maxwell – Boltzmann velocity distribution function along the x direction.

The variation in momentum caused by a molecular impact is $\Delta p = -2mv_x$, as shown in the Figure 3.

Multiplying Δp by the number of impacts given by eqn. 30 and, integrating on positive velocities, the total impulse variation Δp_T^A of the subsystem A results:

$$\begin{aligned} \Delta p_T^A &= -2m \frac{N}{Sx} S \Delta t \int_0^{+\infty} f(v_x) v_x^2 dv_x = \\ &= -2m \frac{N}{Sx} S \Delta t \frac{1}{2} \int_{-\infty}^{+\infty} f(v_x) v_x^2 dv_x = \\ &= -2m \frac{N}{Sx} S \Delta t \frac{1}{2} \langle v_x^2 \rangle_A = -2m \rho_A S \Delta t \frac{1}{2} \langle v_x^2 \rangle_A \end{aligned} \quad (32)$$

where $\langle v_x^2 \rangle_A = \frac{k_B T_A}{m}$ and $\rho_A = \frac{N}{Sx}$ is the numerical density of the subsystem A.

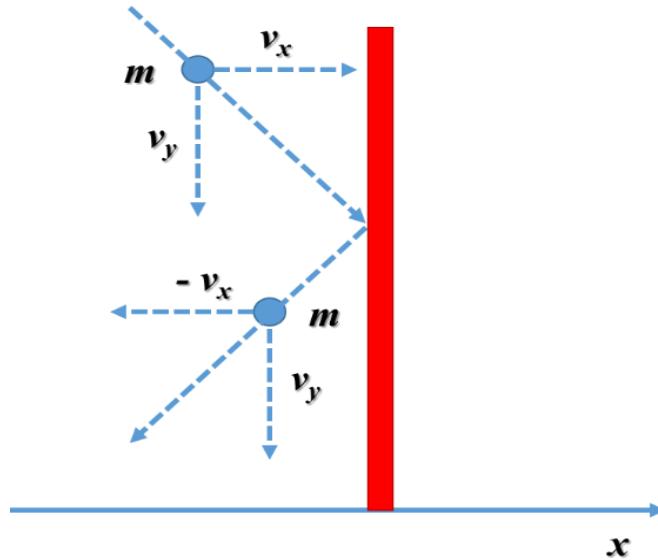


Figure 3. Variation in momentum caused by a molecular impact. The molecule that impacts against the wall perpendicular to the x axis, undergoes a variation of the momentum only with regard to the horizontal component, while the vertical one remains unchanged. One has that $\Delta p = p_f - p_i = \Delta p_x = -mv_x - (mv_x) = -2mv_x$.

Applying the same considerations for system B, one has:

$$\Delta p_T^B = 2m \frac{N}{S(L-X)} S \Delta t \frac{1}{2} \langle v_x^2 \rangle_B = -2m \rho_B S \Delta t \frac{1}{2} \langle v_x^2 \rangle_B \quad (33)$$

where $\langle v_x^2 \rangle_B = \frac{k_B T_B}{m}$ and $\rho_B = \frac{N}{S(L-X)}$ is the numerical density of the subsystem B.

Introducing the infinitesimal work (dL) exerted by the gas:

$$dL = F dx = \frac{dp_T}{dt} dX \quad (34)$$

one has:

$$\frac{dU_A}{dt} = -\frac{dL_A}{dt} = -2m \langle v_x^2 \rangle_A \frac{\rho_A}{2} S dX \quad (35)$$

$$\frac{dU_B}{dt} = -\frac{dL_B}{dt} = 2m \langle v_x^2 \rangle_B \frac{\rho_B}{2} S dX \quad (36)$$

which are equivalent to eqns. 23 and 24.

In the case under examination, the adiabatic piston moves with a velocity v_{piston} given by the eqn. 29; therefore, the number of collisions is:

$$\frac{N}{SX} S v_x \Delta t f(v_x - v_{piston}) dv_x \quad (37)$$

Being the variation of momentum due to molecular impact:

$$\Delta p^A = -2m(v_x - v_{piston}) ; \Delta p^B = 2m(v_x + v_{piston}) \quad (38)$$

Following the same steps previously performed, the new expressions of the work performed by the gas on the piston are obtained:

$$\begin{aligned} nC_v dT_A &= dU_A = -dL_A = \\ -2m \langle \left[|v_x| - \frac{dx}{dt} \right]^2 \rangle \frac{\rho_A}{2} S \frac{dx}{dt} dt &= \\ -m\rho_A S \frac{dx}{dt} \left[\langle v_x^2 \rangle_A - 2\langle |v_x| \rangle_A \frac{dx}{dt} + \left(\frac{dx}{dt} \right)^2 \right] dt &= \\ -m\rho_A S \frac{dx}{dt} \left[\langle v_x^2 \rangle_A - 2\langle |v_x| \rangle_A \frac{dx}{dt} + \left(\frac{dx}{dt} \right)^2 \right] dt & \end{aligned} \quad (39)$$

and, for system B:

$$nC_v dT_B = dU_B = \frac{nRT_B}{L-X} \frac{dx}{dt} dt + \sqrt{\frac{8nRM_g}{\pi}} \frac{\sqrt{T_B}}{L-X} \left(\frac{dx}{dt} \right)^2 dt + m\rho_B S \left(\frac{dx}{dt} \right)^3 dt \quad (40)$$

where it is:

- C_v is the molar heat at constant volume;
- U_A, U_B the internal energies of the two subsystems A and B respectively;
- L_A, L_B the work performed by the gas on the piston;
- $m = \frac{M_g}{N}$ the molecular mass;
- $\rho_A = \frac{N}{SX}$ the number density in subsystem A
- $\rho_B = \frac{N}{SX}$ the number density in subsystem B

- $\langle |v_x| \rangle_A = \sqrt{\frac{2k_B T_A}{\pi m}}$, $\langle |v_x| \rangle_B = \sqrt{\frac{2k_B T_B}{\pi m}}$ the average particle velocities along the x axis (are easily obtained from Maxwell's velocity distribution law);
- $\langle v_x^2 \rangle_A$, $\langle v_x^2 \rangle_B$ the two average quadratic velocities.

With reference to the system energy defined, see eqn. 18, by differentiating both members, with respect to time, and replacing the new expressions of work dL_A and dL_B exerted by the gas contained in the two subsystems on the piston, one obtains a new equation of motion:

$$M\ddot{X} = \left(\frac{nRT_A}{X} - \frac{nRT_B}{L-X} \right) - \sqrt{\frac{8nRMg}{\pi}} \left(\frac{\sqrt{T_A}}{X} + \frac{\sqrt{T_B}}{L-X} \right) \frac{dX}{dt} + M_g \left(\frac{1}{X} - \frac{1}{L-X} \right) \left(\frac{dX}{dt} \right)^2 \quad (41)$$

It is observed that keeping only the first order in $\frac{dX}{dt}$ in eqns. 39 and 40, we find the equations for a reversible adiabatic transformation. Considering the equation of motion defined by eqn. 41, it should be taken into account that the introduction of the piston velocity $\frac{dX}{dt}$ in the momentum conservation law leads to two additional terms, the first of which playing the role of a frictional force. Therefore, once the initial conditions $X_0 = X(0)$, $T_A^i = T_A(0)$ and $T_B^i = T_B(0)$ have been set, the thermodynamic equilibrium state is univocally determined by the asymptotic values X^{as} , T_A^{as} , T_B^{as} of $T_A(t)$, $T_B(t)$ and $X(t)$. Multiplying eqns. 39 and 40 for dt , it is useful to rewrite eqns. 39, 40 and 41 in a dimensionless form, i.e.,:

$$\dot{\Theta}_A = -(\gamma - 1)\Theta_A \frac{\Psi}{\Psi} + \sigma(\gamma - 1)\sqrt{\Theta_A} \frac{\Psi^2}{\Psi} - \frac{\pi}{8}(\gamma - 1)\sigma^2 \frac{\Psi^3}{\Psi} \quad (42)$$

$$\dot{\Theta}_B = (\gamma - 1)\Theta_B \frac{\Psi}{1-\Psi} + \sigma(\gamma - 1)\sqrt{\Theta_B} \frac{\Psi^2}{1-\Psi} + \frac{\pi}{8}(\gamma - 1)\sigma^2 \frac{\Psi^3}{1-\Psi} \quad (43)$$

$$\ddot{\Psi} = \frac{\Theta_A}{\Psi} - \frac{\Theta_B}{1-\Psi} + \sigma \left(\frac{\sqrt{\Theta_A}}{\Psi} + \frac{\sqrt{\Theta_B}}{1-\Psi} \right) \dot{\Psi} + \frac{\pi}{8} \sigma^2 \left(\frac{1}{\Psi} - \frac{1}{1-\Psi} \right) \dot{\Psi}^2 \quad (44)$$

where $\Theta_A = \frac{T_A}{T_a}$, $\Theta_B = \frac{T_B}{T_a}$, $T_a = T_A + T_B$, $\Psi = \frac{X}{L}$, $\tau = \frac{t}{t_\alpha}$, $t_\alpha = \left(\frac{ML^2}{nRT_a} \right)$ and $\sigma = \sqrt{\frac{8Mg}{\pi M}}$ is the motion damping coefficient.

The formulated model allows one to determine the equilibrium values (i.e., the asymptotic values) of T_A , T_B and X , once the corresponding initial values are known.

Numerical solutions of eqns. 42, 43 and 44 for the specific case in which $\gamma = 1,4$ are reported in the Figure 4 for $\Theta_A(0) = 0,9$, $\Theta_B(0) = 0,1$, $\Psi(0) = 0,1$, $\sigma = 0,1$. As noted above, for $\sigma = 0$ the piston oscillates without damping, while for $\sigma \neq 0$ the relaxation time towards equilibrium increases decreasing the value of σ .

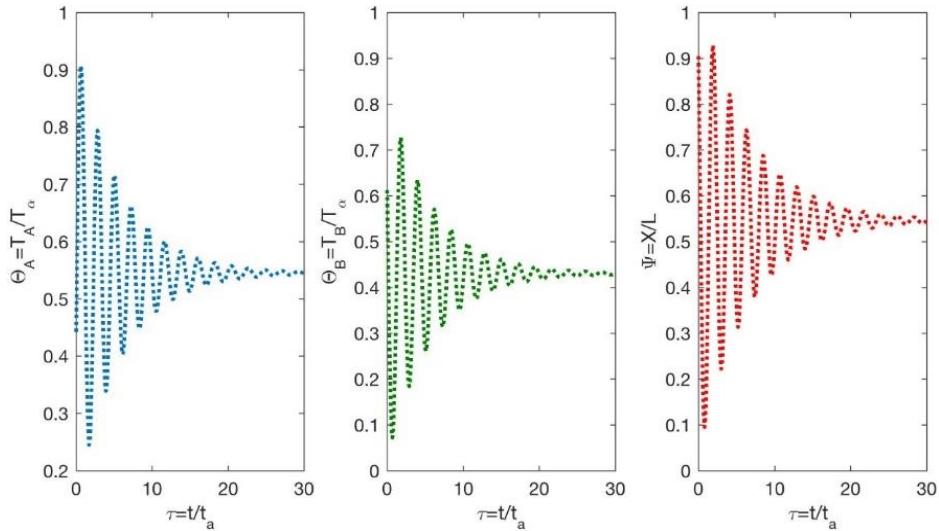


Figure 4. Numerical solutions of eqns. 42, 43 and 44, for a) $\Theta_A(\tau)$, b) $\Theta_B(\tau)$ and c) $\Psi(\tau)$.

Let us now introduce the Wavelet Transform (WT) by defining the general mother wavelet function:

$$\psi_{s,\tau}(t) = s^{-\frac{1}{2}}\psi\left(\frac{t-\tau}{s}\right) \quad (45)$$

where $s > 0$ is the scale parameter and τ represents the shift [10-15]. Such a function has to satisfy two conditions: i) finite energy of the function ψ , and ii) the admissibility condition. Under these conditions, one has:

$$W^y(s, \tau) = \int_{-\infty}^{+\infty} y(t)\psi_{s,\tau}^*(t)dt \quad (46)$$

where $*$ denotes the complex conjugate of ψ . Thus WT allows to decompose a signal $y(t)$, into a set of dilated and shifted mother wavelet functions $\psi_{s,\tau}^*(t)$ [16-22]. WT has been revealed a powerful tool for treating and analyzing in different fields such as medicine, pharmacy, neutron scattering, economics and meteorological. [23-28].

Taking into account two different signals, i.e., $y(t)$ and $h(t)$, by means of WT Cross Correlation (XWT) it is possible to evaluate their degree of similarity at different resolution values. By evaluating $W^y(s, \tau)$ and $W^h(s, \tau)$, it is possible to evaluate the Cross-WT spectrum as:

$$W^{yh}(s, \tau) = W^y(s, \tau)W^h(s, \tau)^* \quad (47)$$

where $*$ denotes the complex conjugate. Due to the complex nature of the coefficients, it is can be written:

$$W^y(s, \tau) = |W^y(s, \tau)| e^{\phi^y(s, \tau)} \quad (48)$$

where the wavelet amplitude is given by $|W^y(s, \tau)|$ and $\phi^y(s, \tau)$ represents the absolute phase. The amplitude and the phase refer to each couple (s, τ) [29-34]. By the Cross-WT power, $|W^{yh}(s, \tau)|$, it is possible to deduce the zones where the two signals have a high common power. Finally, one can calculate the relative phase difference between the two signals:

$$\phi^{hy}(s, d) = \phi^h(s, d) - \phi^y(s, d) \quad (48)$$

In order to highlight the zones where the two signals have a high common power, the XWT approach has been employed, computing also the relative phase difference of the cross-correlation spectrum between the two signals [35-40].

Figure 5 reports the XWT for the numerical solutions 42 and 43. It emerges that the two signals are in anti-phase as it can be inferred by the arrows which point towards the left.

Figure 6 report the XWT for the numerical solutions 42 and 44. In this case the arrows dominantly point towards the left denoting again an anti-phase condition.

Finally, Figure 7 shows the XWT for the numerical solutions 43 and 44. In this case the arrows dominantly point towards the right denoting an in-phase condition.

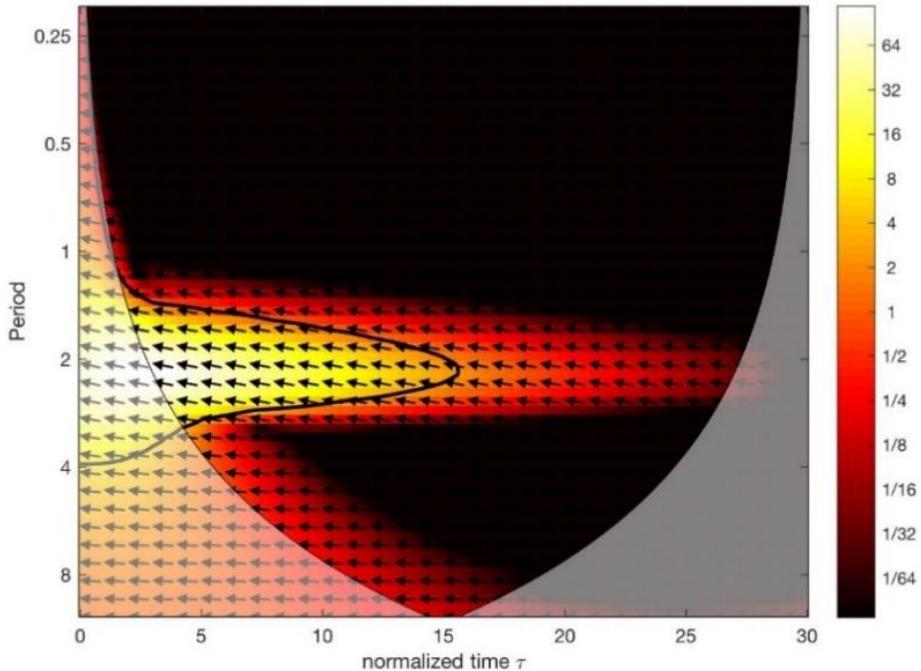


Figure 5. XWT for the numerical solutions 42 and 43 showing that the two signals are in anti-phase.

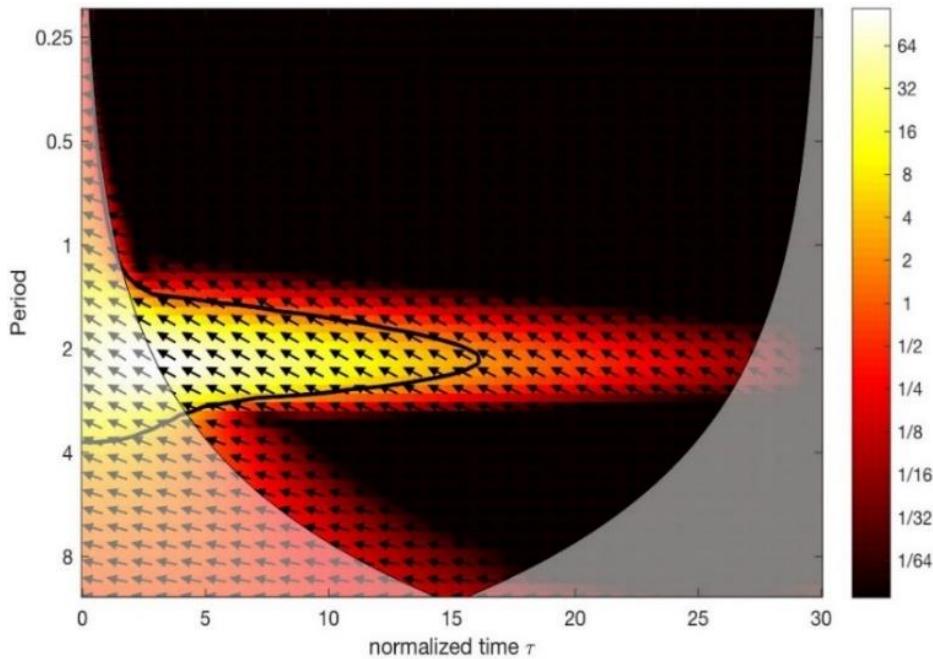


Figure 6. XWT for the numerical solutions 42 and 44. In this case the arrows dominantly point towards the left denoting again an anti-phase condition.

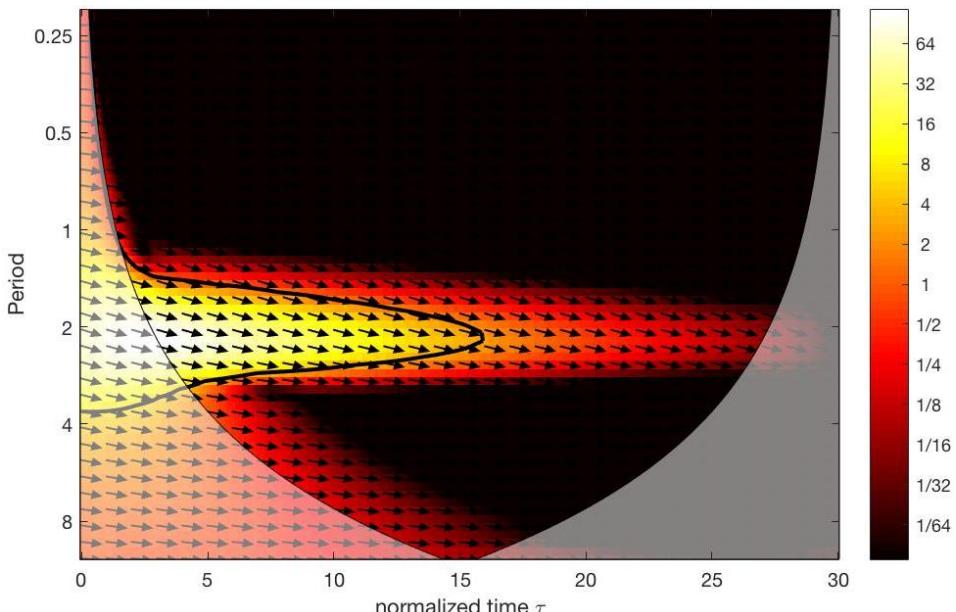


Figure 7. XWT for the numerical solutions 43 and 44. The arrows pointing right denote in-phase spectra.

CALCULATION OF THE ADIABATIC COEFFICIENT γ

The instrument realized “ad hoc” and then employed for the measurement of the adiabatic coefficient γ [41-49] has been designed and built in the Mechanics and Electronics Laboratories of the Department of Mathematics and Computer Science, Physical Sciences and Earth Sciences of the University of Messina (MIFT). It consists of a plexiglass cylinder of volume of about two litres, surmounted by a movable piston. In order to minimize the gas leaks contained inside the plexiglass cylinder, plastic plugs (Darling) have been realized with specific rubber gaskets (O-Rings). Inside the plexiglass cylinder the optical distance sensor, the sensor for measuring the temperature, the barometric sensor a resistance for heating the gas were installed, as shown in Figure 8.

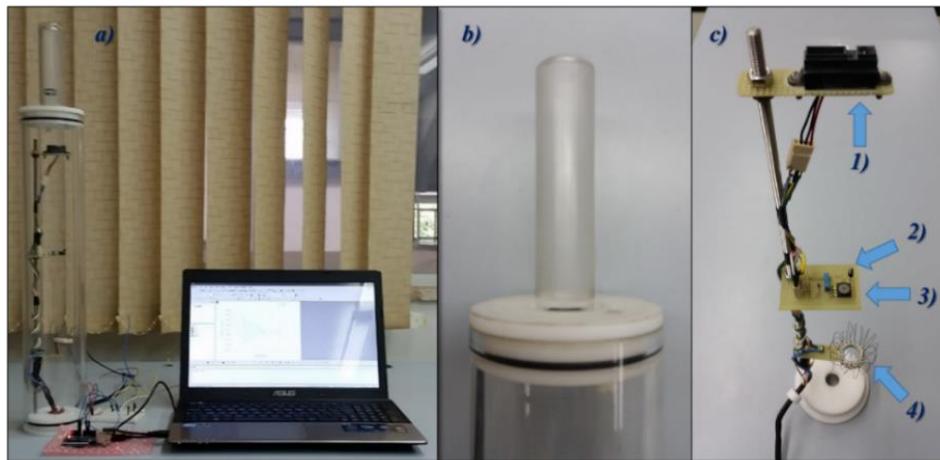


Figure 8. a) Prototype, designed and built entirely in the Mechanics and Electronics Laboratories of the Department of Mathematics and Computer Science, Physical Sciences and Earth Sciences of the University of Messina. It consists of a cylinder of plexiglass of the volume is about two litres, surmounted by a movable piston. b) To guarantee the absence of gas leaks contained inside the plexiglass cylinder, plastic plugs (Darling) have been realized with specific rubber gaskets (O-Rings). c) The optical distance sensor 1), the sensor for measuring the temperature 2), the barometric sensor 3) and a resistance for heating the gas 4) are installed inside the plexiglass cylinder.

The pressure sensor is a sensor on board. The distance sensor is a photoelectric sensor. For its precision and accuracy it is very widespread in the field of robotics. This sensor measures, with a tolerance of 0,5 cm, the distance in the range from 4,0 to 30,0 cm, returning a variable analog value. The temperature sensor is a precision sensor whose output voltage is linearly proportional to the temperature measured in degrees Celsius. It is therefore more advantageous than other the linear temperature sensors calibrated in Kelvin degrees; the obtained result in degrees Celsius is directly derived from the sensor, without the need for further conversions.

Another innovative feature of the employed device is given by the data acquisition system. It is based on the use of an Arduino YUN board, capable of acquiring the fundamental parameters of the experiment through the sensors [50].

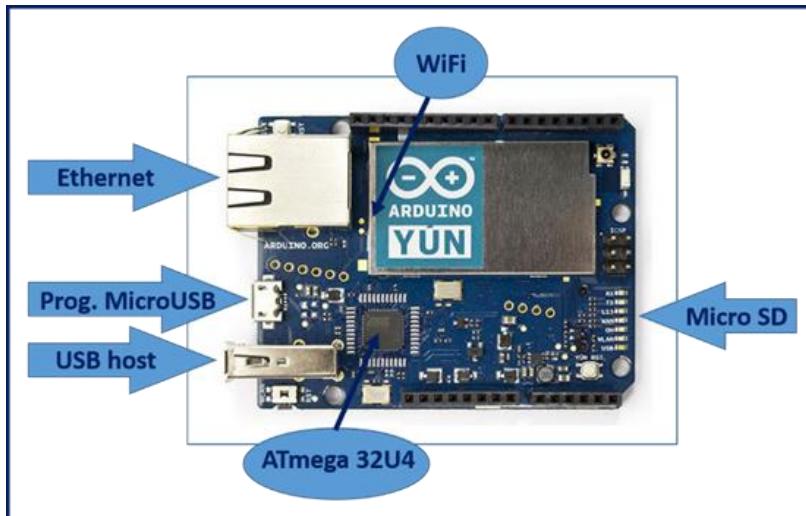


Figure 9. Structure and characteristics of the Arduino YUN board.

The Arduino YUN is a microcontroller board based on the ATmega32u4 and the Atheros AR9331. The board has an Ethernet and WiFi support, a USB-A port, micro-SD card slot and 20 digital pins that can be used as input or output. They operate at 5 volts, can supply or receive a maximum of 40 mA and have an internal pull-up resistor (disconnected by default) of $20 - 50\text{ kOhms}$. In addition to the digital pins, there are 12 analog inputs, labeled A_0 to A_{11} . Each analog input provides 10 bits of resolution (i.e., 1024 different values).

There are 3 reset buttons, one to reset the microprocessor, one to reset the microcontroller and one to reset the WiFi configuration. Finally you can connect peripherals such as USB flash devices to increase memory, keyboards, or webcams.

The programming language used to program the board in this work is the Node.js. It is a framework for implementing server-side applications in Java-Script, which is typically used in client-side applications. The platform is based on the JavaScript Engine V8, which is the Google runtime also used by Chrome and available on major platforms, even if it performs better on UNIX-like operating systems.

The decision to design and use this board is based on the ability to interface with a specially created web page, where all the data collected by the sensors are reported, thus making each experiment accessible to all students of a possible class.

The device allowed to measure the ratio $\gamma = c_p/c_V$ for the air, using a device inspired to the Rüchardt method (1929).

This method exploits the properties of the adiabatic transformations of an ideal gas that follow the equation $PV^\gamma = \text{const}$, where the theory predicts a value for the air $\gamma = 1,4$ being the nitrogen, diatomic gas, the main constituent ($\sim 78\%$).

Starting from following equation:

$$PV^\gamma = \text{const} \quad (49)$$

differentiating one obtains:

$$dP = -\frac{P\gamma}{V} dV \quad (50)$$

Remembering that the pressure is defined as the ratio between the intensity of the pressing force F of a surface and the area of the contact surface A , and replacing dP obtained in the eqn. 50 one has:

$$F = A \cdot \left(-\frac{P\gamma}{V} dV \right) = F = A \cdot \left(-\frac{P\gamma}{V} Ax \right) = -\frac{A^2 P \gamma}{V} x \quad (51)$$

where dV (i.e., the volume's variation) is defined: $dV \cong A \cdot dx$ where dx is the infinitesimal shift and A is the section area. We obtain an equation similar to the strength of a harmonic oscillator ($F = -kx$) where k is a elastic constant and, in this case, is associated with $k = \frac{A^2 P \gamma}{V}$.

In the case in which the friction effects can be neglected, being $k = m\omega^2$ (m = mass e ω = pulsation) one has:

$$\omega^2 = \frac{A^2 P \gamma}{m V} = \left(\frac{2\pi}{T} \right)^2 \quad (52)$$

from which one obtains the period T .

The experiment was carried out by registering the oscillating motion of a movable piston placed on the top of the plexiglass cylinder and, after having measured the period of such oscillations, the γ coefficient was obtained by using the equation:

$$T_R = \frac{2}{r_p^2} \sqrt{\frac{M_p V_c}{\gamma P_c}} \rightarrow \gamma = \frac{4 M_p V_c}{r_p^4 P_c T_R^2} \quad (53)$$

where T_R is the oscillation period, M_p is the mass of the movable piston, P_c is the pressure inside the cylinder, V_c is the volume of the cylinder and r_p is the mobile piston radius.

Figure 10 shows an example of a registered piston oscillation amplitude as a function of time. Figure 11 shows the Fourier transform spectrum that reveals a single peak at 2,65 Hz, to which a period value 0,376 s corresponds.

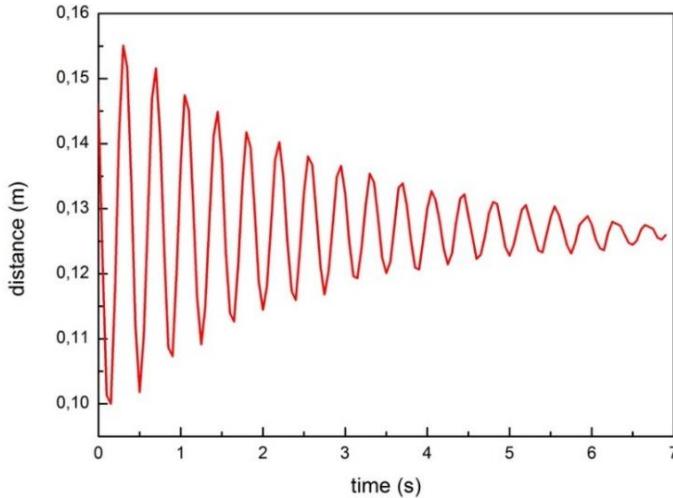


Figure 10. Piston oscillation amplitude as a function of time.

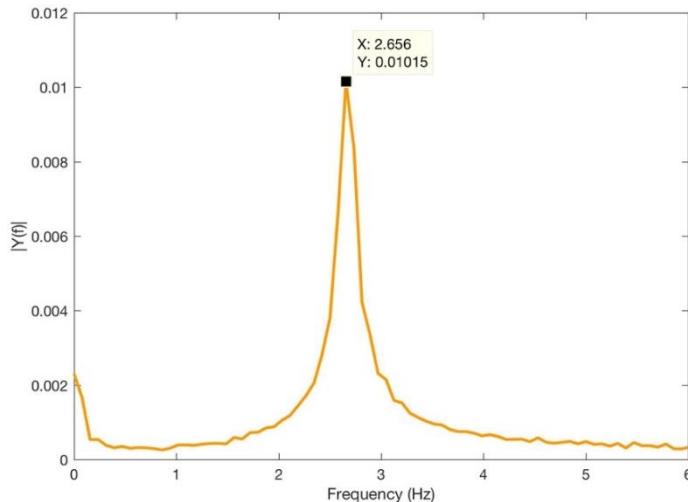


Figure 11. Fourier transform spectrum that reveals a single peak 2,65 Hz.

The set up parameters are the following: mass of the movable piston without metal ring is equal to 89,047 gr.; the volume is 1,930 liters, the average oscillation period is 0,376 s, the square of average oscillation period equals to 0,141 sec², the average of pressure is 994,86 mbar and the radius is 0,014 m. Taking into account all these parameters it is possible to calculate the value of $\gamma = \frac{4M_p V_c}{r_p^4 P_c T_R^2}$ which corresponds to 1,403, value in agreement with that expected for a diatomic gas.

CONCLUSION

The present work reports the main findings of a study addressed to the adiabatic piston problem. The work follows the mental map reported in Figure 12. In particular it is shown how thermodynamics does not provide the univocal solution of the motion problem of the adiabatic piston. If the initial state of the system is defined, thermodynamics only provides the final value of the pressure, whereas the final temperature and volume values can not be derived.

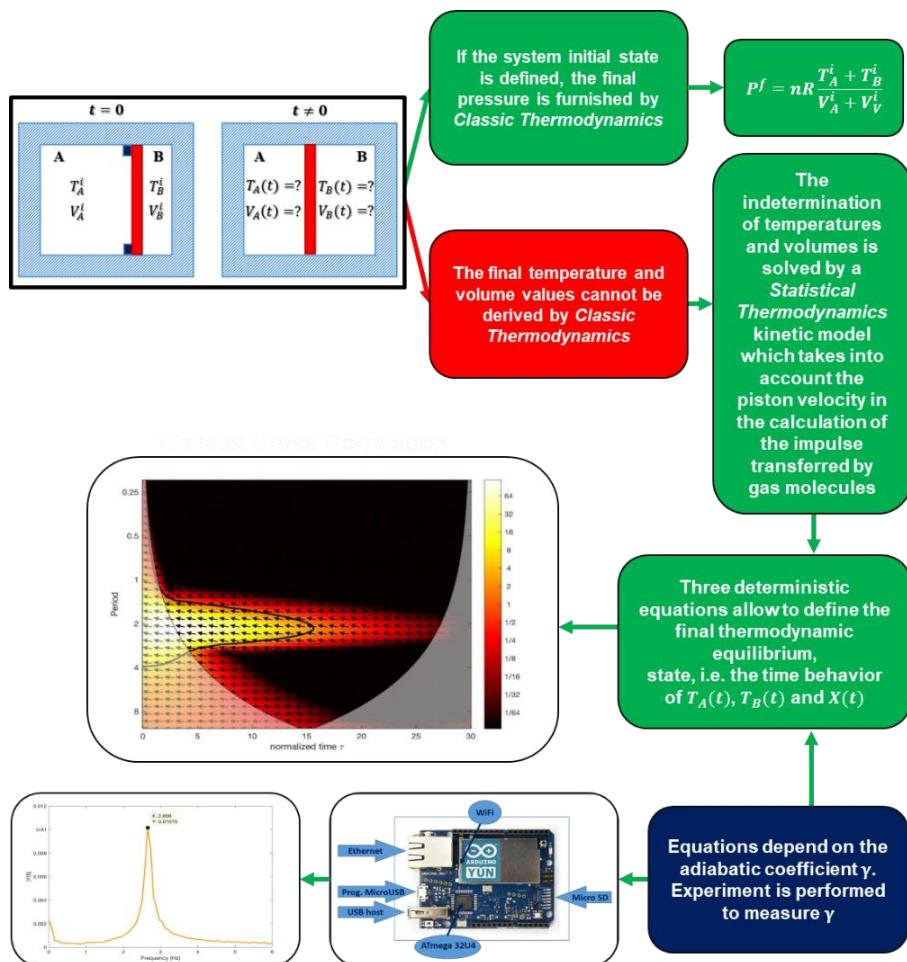


Figure 12. Mental map of the adiabatic piston experience. A simple thermodynamic analysis is not sufficient to univocally determine the final state of the system. The final temperature and volume values are indeterminate. This indeterminacy can be overcome by using an appropriate kinetic model. In the numeric simulation the phase relationships between the temperatures and the piston displacement are shown by applying a Wavelet Cross correlation approach. Finally, the specific gas thermal ratio is evaluated experimentally, through sensors connected to a specifically programmed Arduino board, by measuring the oscillation period of the adiabatic piston and by applying the Fourier transform approach.

The evaution of the final temperature and volume values is performed by meaans of a Statistical thermodynamics kinetic model which takes into account the piston velocity in the calculation of the impulse transferred by gas molecules. In this paper, by means of Wavelet Cross Correlation approach, the phase relations between the temperatures and the piston displacement have been evaluated.

Finally, the specific thermal ratio of the gas is evaluated experimentally by measuring the oscillation period of an adiabatic piston containg air. The oscillation period was calculated using the Fourier transform approach. The relevant physical parameters were collected through sensors connected to a specifically programmed Arduino board.

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Chapter 8

ACOUSTIC STANDING WAVES

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ABSTRACT

In acoustic levitation a standing wave is generated by a piezoelectric crystal which gives rise to a stationary acoustic radiation force. In Physics Education, acoustic levitation furnishes an effective and straightforward method to localize the nodes of acoustic standing waves and to highlight some interesting physical phenomenologies. In the present work two mechanical models to study the damped oscillations of an acoustically levitated sphere are introduced. The work is addressed to graduate Physics, Engineering and Mathematics students.

Keywords: acoustic standing waves, acoustic levitation, damped oscillations, Physics Education, Wavelet Analysis

INTRODUCTION

One of the primary subjects of physics is the concept of waves. Waves are perturbations originated from a source which, although of different nature, have in common the same characteristic equation. The property of the waves to be superimposed

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gives rise, among other things, to the phenomenon of non homogeneous distribution of their energy in space.

Transverse waves are those in which the oscillation occurs in a direction perpendicular to that in which the wave propagates.

In longitudinal waves the oscillation of the medium are parallel to the direction of propagation, as shown in Figure 1.

In gases, such as air, only longitudinal waves propagate, since cohesion effects able to recall the medium towards the equilibrium position are negligible. It should be noticed that, the particles that constitute the medium do not translate but oscillate around their equilibrium position. A wave, therefore, in a strict sense, does not involve the transfer of matter.

In the following the attention will be addressed only to the longitudinal waves and, in particular, to standing acoustic waves that propagate inside an acoustic levitator. It will be shown how particles immersed in acoustic waves are influenced by forces that can be schematized by means of mechanical models constituted by a mass-spring system and by a stretched string.

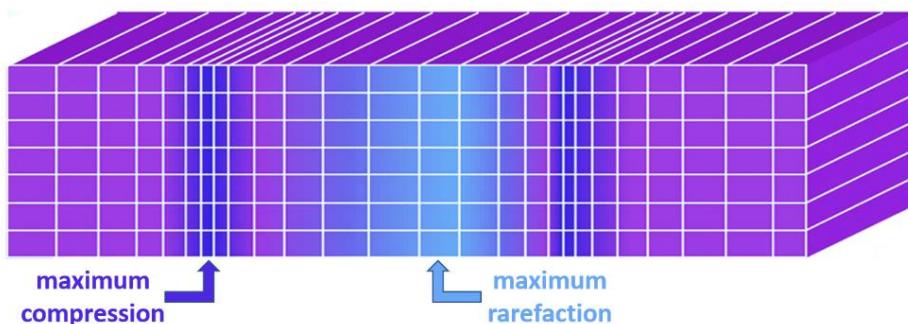


Figure 1. Longitudinal wave in which the oscillations of the medium consist of compressions and rarefactions that occur in the same direction in which the wave propagates.

It should be stressed that in most undergraduate and graduate Physics Education courses, students are usually introduced to the concept of standing waves by means of a discussion on the transverse standing waves on a string. In fact, static images of the standing waves on a fixed string are more easily understood because they show wave patterns corresponding to the transverse displacement of the string.

However, acoustic waves are longitudinal waves and the particle motion associated to a standing acoustic wave, for example in a pipe, is directed back and forth along the pipe axis. In this context, acoustic levitation furnishes an effective and straightforward method to visually show the nodes of acoustic standing waves whose positions are stationary.

Despite standing wave levitation phenomena were first observed in Kundt's tube experiment [1], the first use of acoustic levitation dates back to 1933 [2]. Subsequently,

in 1985 Barmatz and Collas developed techniques that used resonant cavities to create regions that can trap small samples [3]. Figure 2 shows a drawing of the Kundt's tube (denoted inside Figure 2, as Figure 6 and Figure 7) and the powder patterns created by it (denoted inside Figure 2, Figures 1, 2, 3 and 4) [1]. This experimental apparatus allows the measurement of the sound speed in a gas or a solid rod and it was invented in 1866 by a German physicist August Kundt. It is used today only for demonstrating standing waves and acoustical forces.

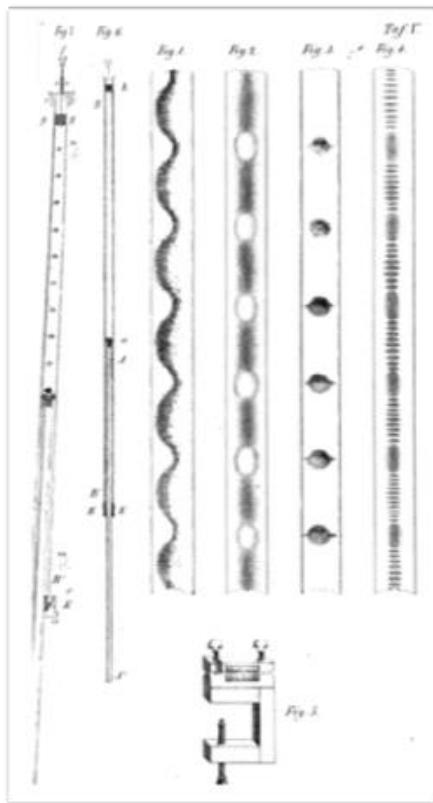


Figure 2. Drawing of the Kundt's tube apparatus (denoted inside Figure 2, as Figure 6 and Figure 7) and the powder patterns created by it (denoted inside Figure 2, as Figures 1, 2, 3 and 4).

In the last years, many levitation techniques [4] have been developed by scientists, for example optical [5-6], electro-magnetic [7-10], electrostatic [11-13], gas-film [14-15], aerodynamic [16-29] and acoustic levitation [30-55].

In many cases levitation is a contactless technique that permits to remove sample-holder interplays and to decrease contamination; furthermore, acoustic levitation is employed for obtaining high concentrations of mixtures starting from solutions. Electric levitation for example is achievable with conductive materials. For these reasons acoustic levitation is widely used in biophysics both for the investigation of aqueous solutions [56-59], disaccharides [60-85], proteins [86-93], polymers [94-138], polyols [139-145],

nano-materials [146-148] and systems of biotechnological interest [149-150]. In particular acoustic levitation is more and more employed in the preparation of highly concentrated mixtures and in conjunction with spectroscopic techniques [151-156].

In this paper, an approach to explain standing waves by means of an acoustic levitator is presented. In particular, it is possible to visually show the nodes of the acoustic standing wave whose positions are stationary; furthermore, two mechanical models to study the damped oscillations of a suspended particle [157-162] are reported, showing as acoustic levitation allows to explain the physical principle of standing waves in an intuitive way.

ACOUSTIC STANDING WAVES

Waves obey to the same differential equation and it is this property that allows to give a unified description. In general, considering a perturbation represented by a function $f = f(x, t)$, the wave equation is:

$$\frac{\partial^2 f}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 f}{\partial t^2} \quad (1)$$

where x is the position, v the velocity of the wave and t the time.

This is a differential equation to partial derivatives, linear of the second order. Solutions of eq. (1) can be written in the form:

$$f = f(x \pm vt) \quad (2)$$

It is relatively simple to prove that eq. (2) is solution of eq. (1), introducing the intermediate variable $s = x \pm vt$. It follows that:

$$\frac{\partial f}{\partial x} = \frac{df}{ds} \frac{\partial s}{\partial x} = \frac{\partial f}{\partial s}, \quad \frac{\partial f}{\partial t} = \frac{df}{ds} \frac{\partial s}{\partial t} = \pm v \frac{df}{ds}. \quad (3)$$

Observing that the derivatives of the function f respect to x and t are obtained by multiplying the derivative respect to s , for 1 and for $\pm v$, it is possible to write:

$$\frac{\partial^2 f}{\partial x^2} = \frac{d^2 f}{ds^2}, \quad \frac{\partial^2 f}{\partial t^2} = v^2 \frac{d^2 f}{ds^2}. \quad (4)$$

Substituting eq. (4) in eq. (1) it is possible to verify that eq. (1) is verified.

The two solutions, $f(x - vt)$ and $f(x \pm vt)$, describe respectively a wave that propagates in the direction of the x axis and in the opposite direction to that of x axis.

A particular case of relevant interest is that in which the source that generates the wave oscillates of harmonic motion, with a fixed pulsation ω . The argument of the wave function must therefore contain, in addition to x and t , also the pulsation ω ; dimensional considerations suggest to express the function in the form:

$$f = A\cos(kx \pm \omega t) \text{ or } f = A\sin(kx \pm \omega t) \quad (5)$$

in which the argument of the trigonometric functions is called “phase.” It is easy to verify that both these functions are solution of eq. (1), as long as exists the relationship:

$$k = \frac{\omega}{v} \quad (6)$$

The parameter k is called “wave number.”

The following relationships are easily verifiable: $v = \frac{\lambda}{T} = \lambda\nu \frac{\omega}{k}$ and $\omega = \frac{2\pi}{T} = 2\pi\nu$.

The phenomenon called “standing waves” occurs when two waves of the same nature and of the same frequency propagate in the same medium in opposite directions and they overlap.

Sound is a longitudinal pressure wave, constituted by the alternation of compressed and rarefied air layers. Considering a long tube, full of air, closed at one end by a piston that can slide back and forth. As the piston advances, it compresses the volume of air adjacent to it; consequently, the air pressure contained in that volume increases and the air tends to expand from both sides, compressing the next volume of air and at the same time restoring the previous pressure from the piston side; in this way the impulse produced by the piston is transmitted along the tube (see Figure 3).

If the piston moves in the opposite direction a pressure vacuum is created.

Figure 4 shows what happens to a sphere volume at different times, as a rightward-traveling wave passes by. The darker regions indicate higher pressure and density zones, whereas the lighter regions indicate lower pressure and density zones.

In the 1st case, the sphere volume is located at its equilibrium position (indicated by the vertical blue line) moving towards the right side with maximum velocity; at this position the pressure and density take the maximum value too while the net force is zero. In the 2nd case, the sphere volume is decelerating due to the pressure which is higher on the right than on the left particle side. In the 3rd case, the sphere value is at its maximum displacement and acceleration, while its velocity is zero. In the 4th case it is moving leftward while in the 5th case, it crosses the equilibrium position with the maximum negative velocity.

For an acoustic wave, intensity is defined as the energy carried by the wave per unit area and per unit of time.

The human ear can be considered as a sensitive receiver with the ability to perceive sounds whose intensity varies in a large interval. Ear response has a particular non-linear characteristic curve; it does not produce a double sound sensation when it doubles the objective intensity of the pressure wave, but has a logarithmic response. The ear response also depends on the sound frequency as shown in Figure 5. Each of the graph curves refers to sounds of different frequencies that generate the same sound sensation. The set of all isophonic curves defines the field of audibility.

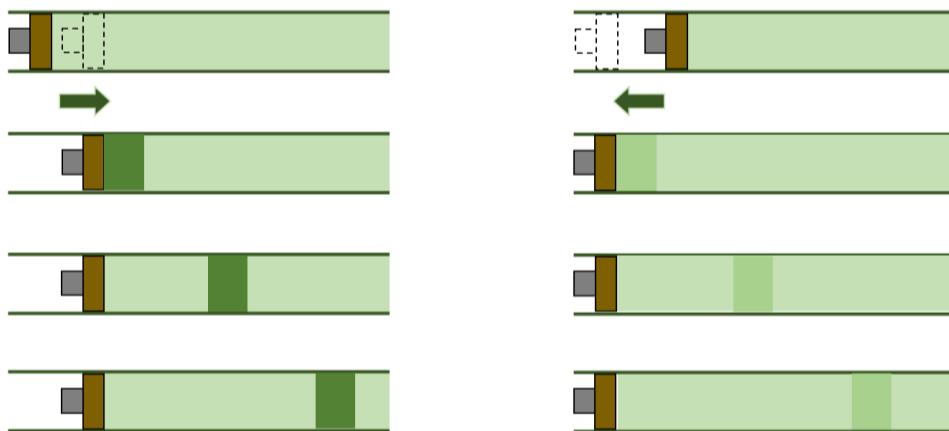


Figure 3. Longitudinal pressure wave, constituted by the alternation of compressed and rarefied air layers, represented by a long tube, full of air, closed at one end by a piston that can slide back and forth.

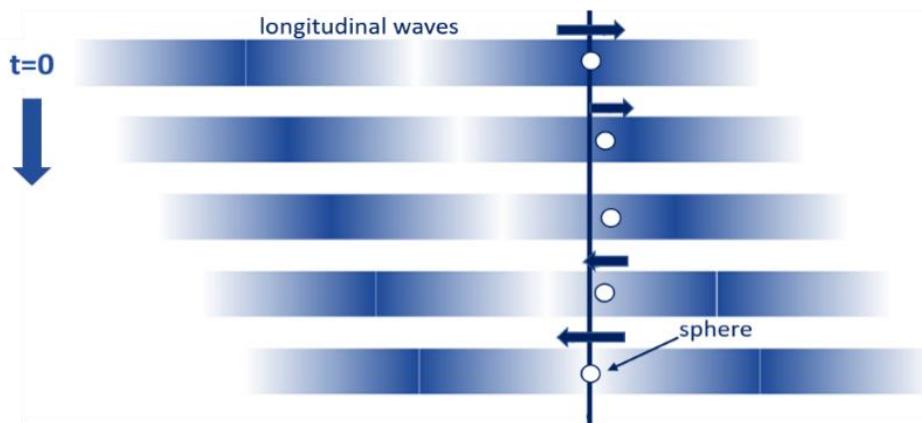


Figure 4. Half cycle of a sphere volume at a few different times, as a rightward-traveling wave passes by.

Acoustic waves which can be perceived by the human ear have a frequency between 20 Hz and 20 KHz; below 20 Hz the waves are called “infrasonic” and above the 20 KHz “ultrasonic” (see Figure 5). The lower curve refers to the threshold of audibility, the highest one indicates the pain threshold (loudness level), at the frequency of 1000 Hz; they correspond respectively to 10^{-12} W/m^2 and 1 W/m^2 .

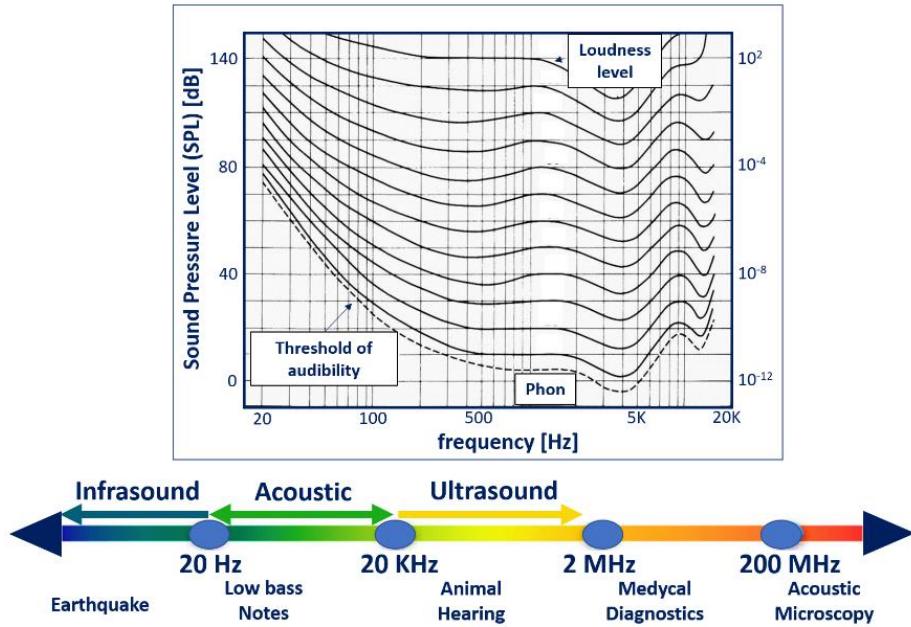


Figure 5. Field of audibility (upward). Sound range diagram (below), from infrasounds to ultrasounds. Acoustic waves perceived by human ear span, with a different weight, from 20 Hz to 20 KHz.

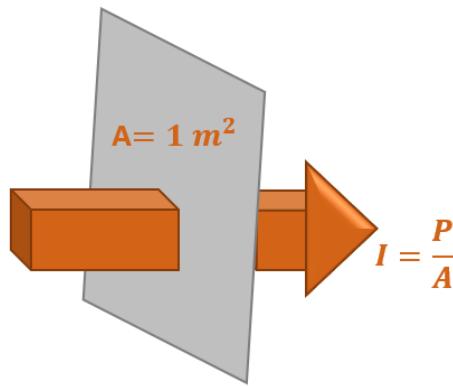


Figure 6. Intensity of a sound wave I that pass through a surface $A = 1 \text{ m}^2$.

The intensity of a sound wave I is the energy that it carries in the unity of time through a surface of 1 m^2 placed perpendicular to the direction of propagation of the wave (see Figure 6).

It is therefore a power per unit of surface and its measure unit is W/m^2 :

$$I = \frac{E}{\Delta t \cdot A} = \frac{P}{A} \quad (7)$$

This definition adapts to any type of wave; from it derives an important property of the energy transmission through the waves. It is such as a small sound source that emits

with the same intensity in all directions (isotropic source) and it considers the energy that flows inside a pyramid that has as vertex the source (see Figure 7).

From the definition of I follows: $I_1 = \frac{P}{A_1} = \frac{P}{l_1^2}$ and $I_2 = \frac{P}{A_2} = \frac{P}{l_2^2}$ from which it derives: $\frac{I_2}{I_1} = \frac{l_2^2}{l_1^2}$. Figure 7 shows that the triangles of vertex O and basis l_1 and l_2 are similar, so derives that: $\frac{l_1}{l_2} = \frac{d_1}{d_2}$. Substituting it in the previous equation it is possible to obtain: $\frac{I_2}{I_1} = \frac{d_1^2}{d_2^2}$ that is the inverse square law of distance.

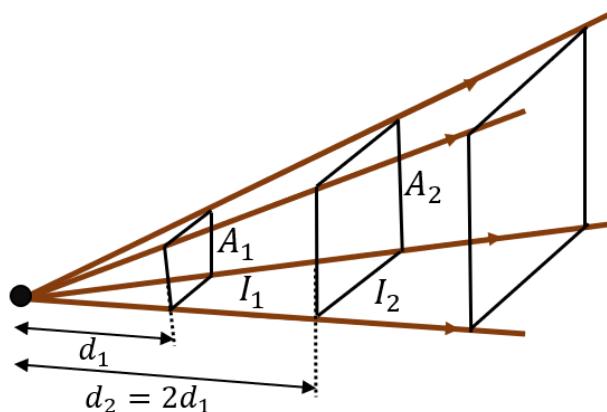


Figure 7. Wave propagation follows the inverse square law of distance.



Figure 8. Standing waves in an acoustic levitator which furnish stable equilibrium locations for levitated particles.

Therefore, the wave intensity, emitted by an isotropic source, decreases with the inverse of the square of the distance from the source.

When an acoustic wave reflects off of a surface, the interaction between its compressions and rarefactions induces interferences, that can combine to create a standing wave. Standing acoustic waves have defined nodes, i.e., areas of minimum pressure, and antinodes, i.e., areas of maximum pressure.

Figure 8 shows the stable equilibrium locations for levitated particles.

Two different kinds of waves are employed in acoustic levitation to generate acoustic radiation pressure, they are defined as traveling waves or Near-field Acoustic Levitation (NFAL) and standing waves or Standing Wave Acoustic Levitation (SWAL) (see Figure 9).

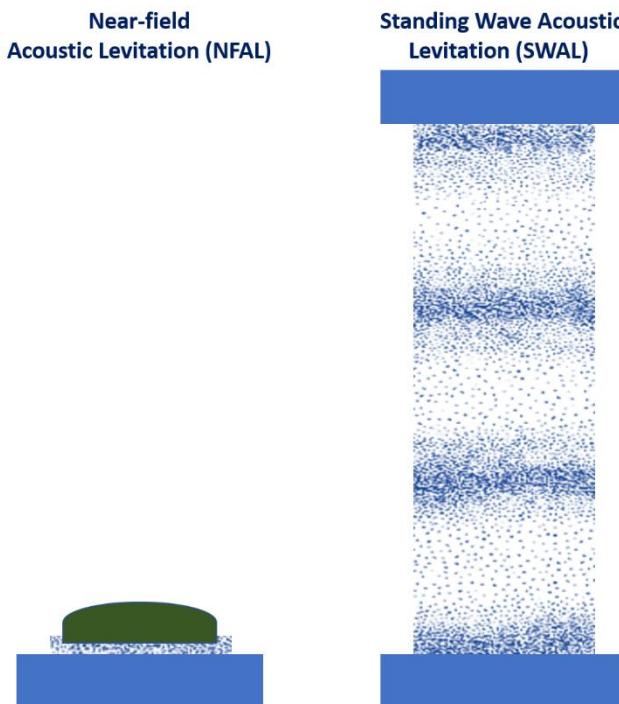


Figure 9. Two different kinds of waves are employed in acoustic levitation to generate acoustic radiation pressure: traveling waves or Near-field Acoustic Levitation (NFAL) (on the left) and standing waves or Standing Wave Acoustic Levitation (SWAL) (on the right).

The first ones propagate through a medium with transport of energy, the second are stationary waves, generated by two traveling waves, an incident and a reflected wave. They present pressure nodes, i.e., positions where the pressure is zero and antinodes, in which the pressure fluctuates between a maximum and minimum value.

In NFAL, samples are levitated and transported at a very small distance above a vibrating surface using ultrasonic Surface Acoustic Waves (SAW)s by means of squeeze film effects in near field.

In SWAL, small samples of different shape are levitated in pressure nodes. The acoustic radiation force limits the sample weight. A typical SWAL design, which has one transducer and one reflector, creates a standing wave as shown in Figure 10, where the acoustic radiation pressure balances the gravity.

Waves, produced by a transducer and a reflector present pressure nodes and anti-nodes along the blue vertical line. A sample is trapped at a pressure node because of the time-averaged forces of the acoustic radiation pressure. These forces at pressure antinodes push the object axially. The sample is located slightly below a pressure node due to the gravitational force. In Figure 11, a representation of the acoustic force, the pressure wave and the acoustic potential is reported. The period of the pressure wave is twice of that of the acoustic force wave.

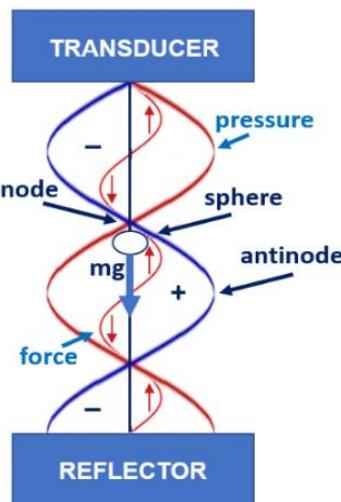


Figure 10. Particle suspended inside an acoustic levitator.

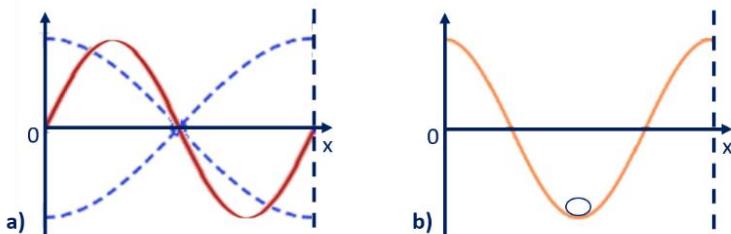


Figure 11. a) Sketch of the acoustic force (solid red line) and the pressure wave (dashed blue line) and b) the acoustic potential (solid orange line).

In an acoustic levitator, a standing wave is generated by a piezoelectric crystal which gives rise to a stationary acoustic radiation force when the distance between two transducers is an integral multiple of the half wavelength.

The transducers, made of aluminum alloy, are driven by piezoelectric drivers, inside an aluminum mounting tubes of 38 mm diameter. The nominal frequency of the transducers is 22 KHz. The distance of the two transducers is set to a nominal separation of 10 acoustic wavelengths, approximatively 150 mm. Two acoustic absorbing foam disks approximately 50 mm in diameter are glued onto the face of the transducer horns to reduce unwanted reflections that can cause instabilities in the levitated sample.

For a perfect gas, the equation of state, known as ideal gas law, is:

$$PV = nRT \quad (8)$$

In an adiabatic process, pressure P is a function of density ρ :

$$P = C\rho \quad (9)$$

where C is a constant.

Pressure and density can be divided into mean and total components: $C = \frac{\partial P}{\partial \rho}$:

$$P - P_0 = \left(\frac{\partial P}{\partial \rho}\right) (\rho - \rho_0) \quad (10)$$

The adiabatic bulk modulus for a fluid is defined as:

$$B = \rho_0 \left(\frac{\partial P}{\partial \rho}\right)_{adiabatic} \quad (11)$$

which give the result:

$$P - P_0 = B \left(\frac{\rho - \rho_0}{\rho_0}\right) \quad (12)$$

Condensation, s , is defined as the change in density for a given ambient fluid density.

$$s = \frac{\rho - \rho_0}{\rho_0} \quad (13)$$

The linearized equation of state becomes: $p = B_s$, where p is the acoustic pressure $(P - P_0)$.

The continuity equation for the conservation of mass is:

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial x} (\rho u) = 0 \quad (14)$$

where u is the flow velocity of the fluid. The equation can be linearized and the parameters can be divided into mean and variable components, as following:

$$\frac{\partial}{\partial t}(\rho_0 + \rho_0 s) + \frac{\partial}{\partial x}(\rho_0 u + \rho_0 s u) = 0 \quad (15)$$

Considering that ambient density changes with neither time nor position and that the condensation multiplied by the velocity is a very small number:

$$\frac{\partial s}{\partial t} + \frac{\partial}{\partial x} u = 0 \quad (16)$$

Euler's force equation for the conservation of momentum is:

$$\rho \frac{D u}{D t} + \frac{\partial P}{\partial x} = 0 \quad (17)$$

where D/Dt is the convective, substantial or material derivative.

From the linearization of the variables:

$$(\rho_0 + \rho_0 s) + \left(\frac{\partial}{\partial t} + u \frac{\partial}{\partial x} \right) u + \frac{\partial}{\partial x} (P_0 + p) = 0 \quad (18)$$

Neglecting small terms, the equation becomes:

$$\rho_0 \frac{\partial u}{\partial t} + \frac{\partial p}{\partial x} = 0 \quad (19)$$

Considering the time derivative of the continuity equation and the spatial derivative of the force equation results in:

$$\frac{\partial^2 s}{\partial t^2} + \frac{\partial^2 u}{\partial x \partial t} = 0 \quad (20)$$

$$\rho_0 \frac{\partial^2 u}{\partial x \partial t} + \frac{\partial^2 p}{\partial x^2} = 0 \quad (21)$$

and multiplying the first by ρ_0 , subtracting the two and substituting the linearized equation of state, it becomes:

$$-\frac{\rho_0}{B} \frac{\partial^2 P}{\partial t^2} + \frac{\partial^2 p}{\partial x^2} = 0 \quad (22)$$

The result is:

$$\frac{\partial^2 p}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 P}{\partial t^2} = 0 \quad (23)$$

where $c = \sqrt{\frac{B}{\rho_0}}$ is the speed of propagation.

The solution of eq. (22), can be found as:

$$p = p_0 \sin(kx) e^{-i\omega t} \quad (24)$$

where p_0 is the pressure amplitude, $k = \omega/c_0$ the wave number, ω the angular frequency and a pressure node located at $x = 0$ is the boundary condition.

Spheres of different diameter and weight, can levitate in the pressure nodes; these nodes and anti-nodes appear at fixed points separated by a distance of $\lambda/2$. Knowing the frequency of the transducer, $f = 22\text{KHz}$ and the velocity sound, $v_s = 343\text{m/s}$ at the considered temperature $T = 22^\circ\text{C}$, it is possible to determine the wavelength of the standing wave as it follows:

$$\lambda = \frac{v_s}{f} = \frac{343000}{22000} = 1,56\text{cm} \quad (25)$$

In Figure 12, the forces that are responsible for compensating the gravitational force and that hold the sample in the pressure node, are sketched.

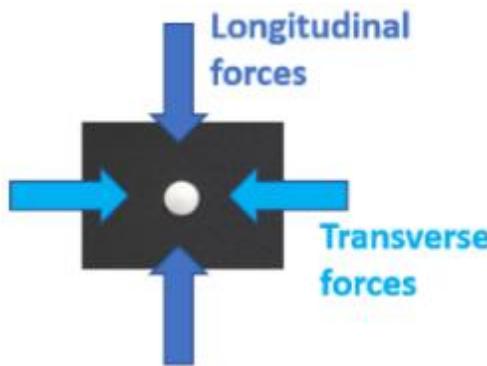


Figure 12. Levitation forces that are responsible for compensating the gravitational force and that are able to levitate the particle.

An object in the presence of a sound field will experience forces associated with the field. An acoustic force arises from the scattering of the sound wave by the body. In order to have an object suspended in the acoustic field, the acoustic force should counteract the gravity force, i.e., weight of the object.

MECHANICAL MODELS FOR MOTION OF AN ACOUSTICALLY LEVITATED SPHERE

Two mechanical models will be introduced to study the damped oscillations and the motion of an acoustically levitated sphere around the node. They represent respectively longitudinal and transverse forces and are constituted by a mass-spring system and by a stretched string.

In principle, an acoustic levitator is a system in which a transducer produces an impulse, characterized by a wave-form that permits to a sample to levitate, but in unstable condition. It can be dealt as a mechanical equivalent model, constituted by a mass-spring system of elastic constant k , connected to a mass m (see Figure 13).

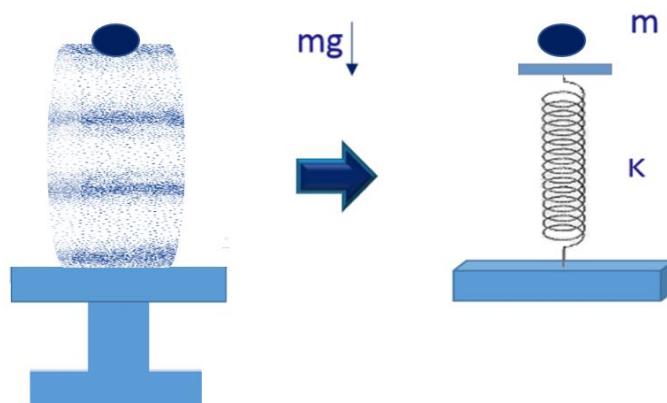


Figure 13. Mass-spring system of elastic constant k to study the damped oscillations of a mass around a node (longitudinal forces).

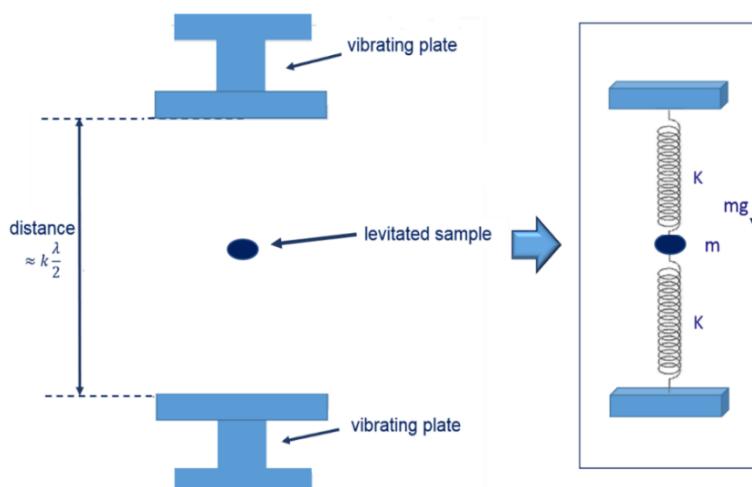


Figure 14. Mass-spring system of elastic constant $2k$ to study the damped oscillations of a mass around a node.

A mechanical model to study the damped oscillations of a mass around a node is constituted by two springs of equal elastic constant k , connected to the mass m and is shown in Figure 14. The system can be simplified in a single mass-spring system of elastic constant $2k$. The equation of the system is the following second-degree differential equation:

$$m\ddot{y} + \gamma_L \dot{y} + 2kx = -mg \quad (26)$$

in which m is the mass, γ_L the longitudinal damping coefficient, k the elastic constant, g the gravity acceleration, $F = -mg$ the force weight, y describes the position, \dot{y} and \ddot{y} are respectively the first and second derivative of y . The solution of the equation is constituted by the sum of a solution in t , $y_h(t)$ and a particular solution, y_p :

$$\begin{cases} y_h(t) = A_L e^{-\frac{\gamma_L t}{2}} \sin(\omega_L t + \varphi) \\ y_p = -\frac{mg}{2k} \end{cases}$$

with $\omega_L = \sqrt{\frac{2k}{m}}$ pulse or angular frequency, measured in [rad/s]. So, the solution of the equation became:

$$y(t) = A_L e^{-\frac{\gamma_L t}{2}} \sin(\omega_L t + \varphi) - \frac{mg}{2k} \quad (27)$$

The second mechanical model is employed to study the damped oscillations of a mass around the node (transverse forces, as shown in Figure 15).

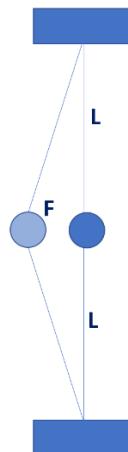


Figure 15. Stretched string to study the damped oscillations of a mass around a node.

Considering a mass m , connected to two equal stretched strings of length L , on which a tension T acts. If the mass is moved of a small step x in the horizontal direction, assuming that the tension T not varies appreciably, it is possible to obtain that the recall force is equal to: $F = -\left(\frac{2T}{L}\right)x$.

So, the equation of the system became in this case:

$$m\ddot{x} + \gamma_T \dot{x} + \left(\frac{2T}{L}\right)x = 0 \quad (28)$$

in which m is the mass, γ_T the transverse damping coefficient, k the elastic constant, T the tension on the two stretched strings, L the length, x describes the position, \dot{x} and \ddot{x} are respectively the first and second derivate of x . The solution of eq. (28) is:

$$x_h(t) = A_T e^{-\frac{\gamma_T t}{2}} \sin(\omega_T t + \varphi) \quad (29)$$

where for the pulsation is: $\omega_T = \sqrt{\frac{2T}{mL}}$.

RESULTS AND DISCUSSION

The results of the damped oscillations of an acoustically levitated sphere of 4 mm of diameter and 2,19 mg of weight are discussed in this section. The measurements were performed, considering for the two transducers an instrument (SAL™ Materials Development Inc.) *Amplitude control*, A, ranging between 3,5 and 6,25 and a frequency of 22 KHz. In the following, only the study with A equal to 6 is reported. The initial amplitude of the oscillation was set-up by approaching the sphere with a wood stick.

Figure 16 shows the measured signal and the fitting result performed by using the following formula:

$$s(t) = 0.7e^{-2.5t} \sin(2\pi \cdot 6.289t) \quad (30)$$

As it can be seen from the figure, significative oscillations occur within about 1,56 s; these oscillations are to be connected with the acoustic transverse forces.

In order to investigate the dependence of oscillation frequency on the instrument *Amplitude control*, A, different measurements were performed by varying A between 3,50 and 6,25. The results are reported in Figure 17.

Finally, a dynamic measure was performed by varying in time the instrument *Amplitude control*, A, and hence the pulsation of the signal. Figure 18 shows the time behavior of $\omega(t)$.

In order to analyze the frequency variation of the registered signal, in the following we perform a comparative Fourier and Wavelet analysis [163-172].

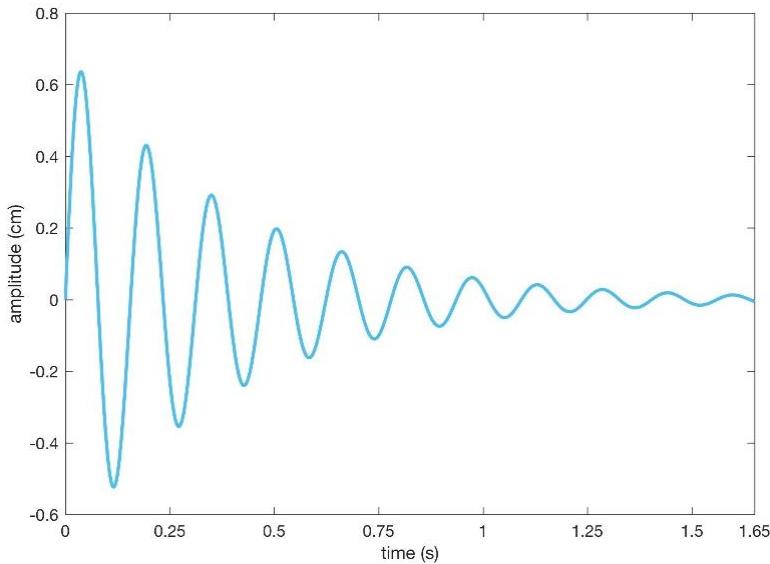


Figure 16. Registered signal of the transversal motion of an acoustically levitated sphere of 4 mm of diameter and 2,19 mg of weigh.

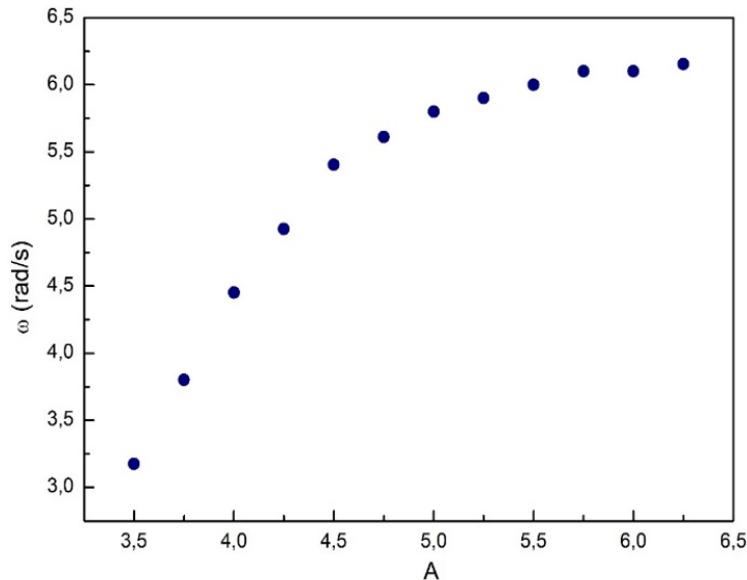


Figure 17. Dependence of the pulsation of the signals on instrument *Amplitude control*, A, when it increases between 3,50 and 6,25.

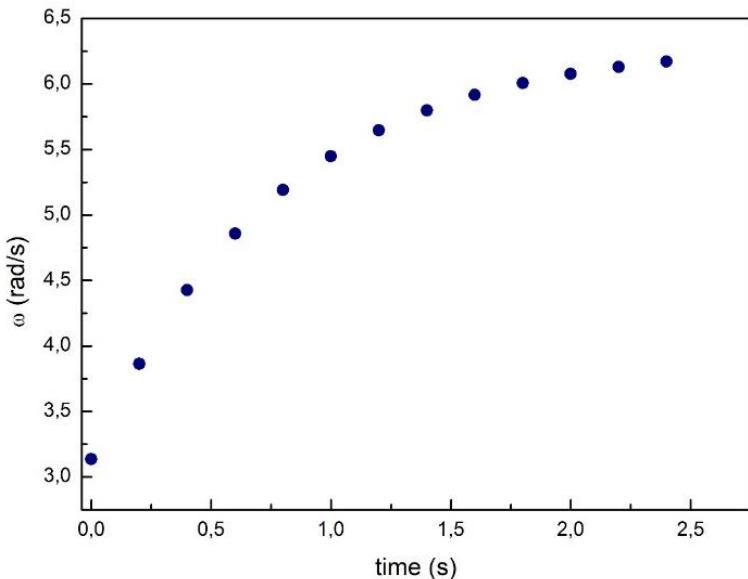


Figure 18. Pulsations of the analyzed signal that vary as a function of time following a square root trend.

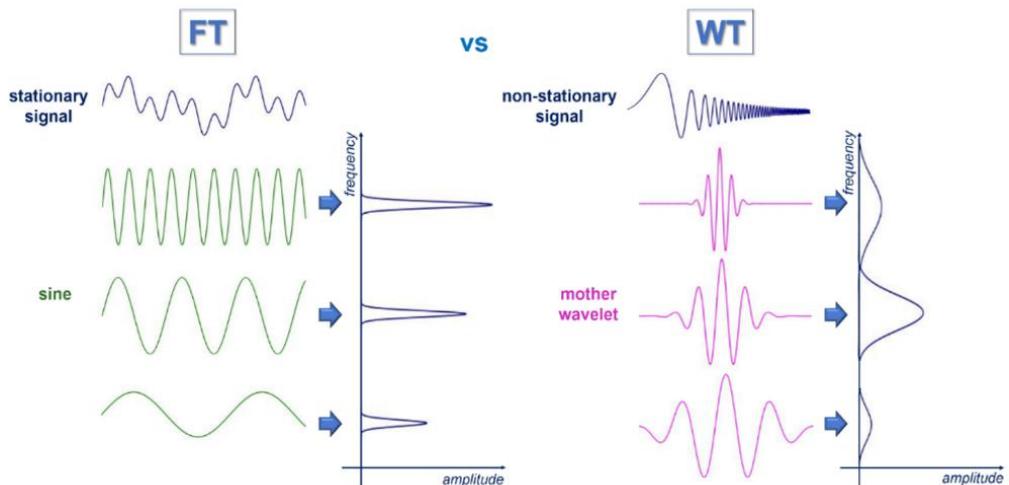


Figure 19. Comparison between Fourier Transform (FT) and Wavelet Transform (WT).

Figure 19 shows a comparison between the Fourier Transform (FT) and the Wavelet Transform (WT). In particular on the left, FT decomposes a stationary signal $f(t) = \sin(0.5t) + \sin(t) + \sin(3t)$ into three sinusoids of different frequencies, which sum to the original waveform; here the spectral power identifies their respective amplitudes.

In contrast to the FT, WT can be considered locally periodic wave-trains. As shown on the right of Figure 19, a family of wavelets is obtained by shifting and scaling a

prototype mother wavelet, such that this set of functions adequately sample all the frequencies present in the non-stationary signal. All these wavelets present the same number of cycles for different frequency bands and they result in different wavelet durations. The convolution gives time-varying amplitudes of the signal in frequency and time, because it expresses the amount of overlap between the signal and this family of functions.

Figure 20 shows on the top the registered signal together with the WT scalogram and FT spectrum. In particular it is shown how WT allows to follow the square root trend of the pulsations as a function of time.

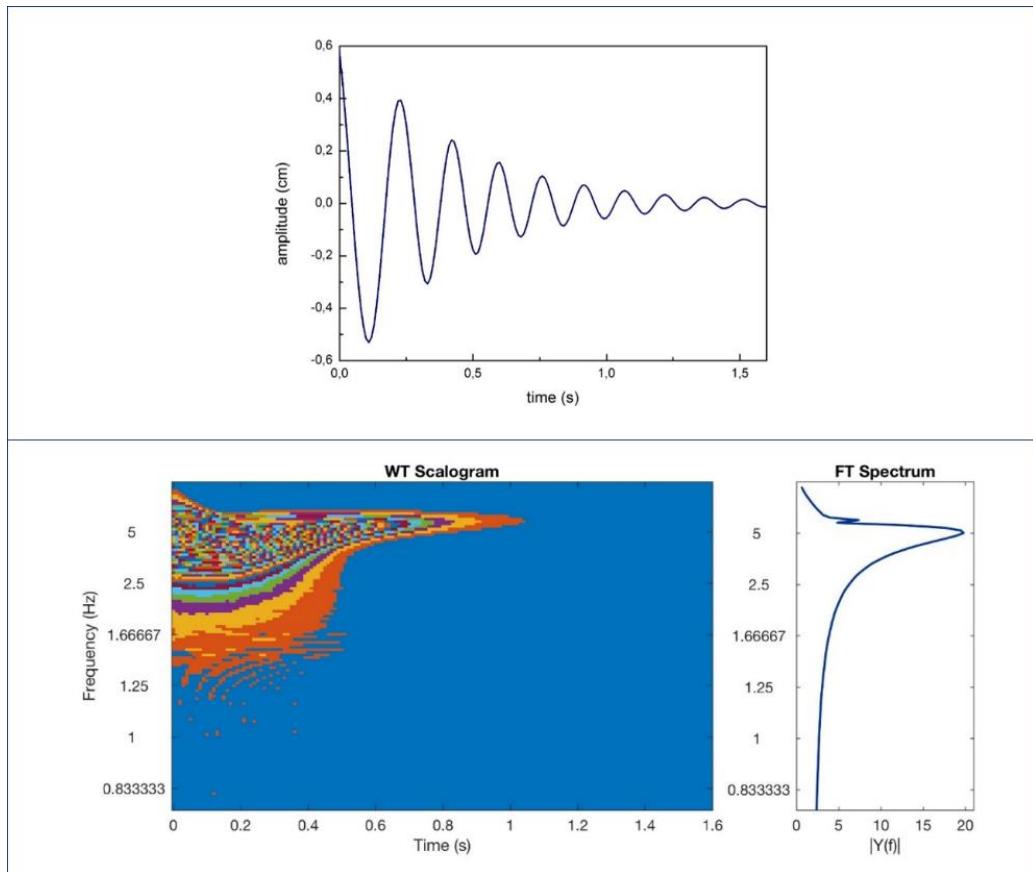


Figure 20. Registered signal (on the top); WT scalogram and FT spectrum.

From the WT and FT analysis it is possible to follow the trend of the pulsations of the analyzed signal as function of time. The obtained results show in an effective way that by increasing the amplitude value the oscillation frequency of the levitated particle increases.

CONCLUSION

In this paper, an approach to explain the standing waves by means of an acoustic levitator is presented. In particular, thanks to the employment of an acoustic levitator, an effective and straightforward method to visually show the nodes of acoustic standing waves is shown. Two mechanical models to study the damped oscillation of a sphere around a single node are introduced. By means of the WT analysis it is possible to follow the trend of the pulsations of the analyzed signal as function of time. The obtained results show in an effective way that by increasing the instrument Amplitude control value the oscillation frequency of the levitated particle increases.

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Chapter 9

METEOROLOGICAL MAPS: HOW ARE THEY MADE AND HOW TO READ THEM. A BRIEF HISTORY OF THE SYNOPTIC METEOROLOGY DURING THE LAST THREE CENTURIES

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ABSTRACT

Meteorology is an interdisciplinary science, which uses the laws of physics, mathematics and chemistry to simplify the understanding of the process occurring in the Earth's atmosphere.. One of the most widespread and used ways of representing meteorological products is definitely that of maps. Millions of people consult the different types of existing weather maps on a daily basis. Most of users do not know how the maps are created nor the exact meaning of the symbols represented in it. The purpose of this paper is to try to answer all these questions. In order to better understand the topic, we will start from the description of the history of meteorology during last 300 years, up to the description of the modern methods of production of the maps, by means of computer and specific software.

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Keywords: synoptic meteorology, meteorological maps, history, analysis, weather forecast

1. INTRODUCTION

It is well known that Meteorology is a highly interdisciplinary science that by means of the laws of physics, mathematics and chemistry allows to understand the atmosphere of the Earth together with its processes and its structure.

Since ancient times, ancient civilizations observed and recorded weather conditions in order to support the agricultural activity and, also, to satisfy own curiosity about the world. In particular, over the centuries the atmosphere has been object of study for different purposes, such as agriculture, military defense and early warnings for severe weather systems like tornadoes and hurricanes. Thanks to the scientific computing development and to an increase of the total number of meteorological observations in a day, it has been possible to improve the forecasts and to better understand the atmosphere [1].

Nowadays, more than a billion people use meteorology by means of countless smartphone apps, which allows them to know with a week in advance, the weather forecast at any location on Earth. Other thousands of people on the ground, on board ships or flying on airplanes, use the most sophisticated and complete meteorological products that are meteorological maps. Apart from rare exceptions, anyone at least once in their life has had to deal with a weather map. The main television channel broadcasting meteorological programs and weather forecasts, do so using and showing to their audience simple meteorological maps, which are able to transmit the information, in an easy and immediate way, to an audience not always sufficiently literate. In the USA there is even a television channel (The Weather Channel) devoted entirely to weather forecasts on which, 24 hours a day, are alternated valid weather forecast for every corner of the World and documentaries on meteorology. This enormous pervasiveness of meteorology and its applications in the life of most of the inhabitants of the planet is opposed to a poor understanding of weather phenomena and the laws that lead the Atmospheric Sciences. The aim of this paper is to explain what a meteorological map is, what information it contains and how it is done. Moreover, it is explained which and how much data are needed to produce a meteorological map, how these data are collected from the various meteorological stations distributed on the earth's surface and finally how these collected data are plotted and represented on the maps.

2. A LITTLE HISTORY

2.1. Galileo and the Court of Ferdinand II

In a cultural and political environment dominated by forms of absolutism, the European science of seventeenth century, opened with the extraordinary figure of Galileo Galilei. Astronomer, mathematician and physicist of recognized standing. The great scientist opposed a methodology based on tangible observation of natural phenomena and the consequent verification by means of suitably programmed experiments of the assumptions arose from the observation itself to the conception of science that was until then based on abstract deduction and blind obedience to the authority of the philosophers of which notably Aristotele. It is the beginning of the experimental method and the overcoming of the boundary line between the ancient and modern science. In the field of meteorology, the first relevant result of Galileo innovative quantitative science was undoubtedly the invention, refinement, and the subsequent use of main measuring instruments such as thermometer, barometer, hygrometer and rain gauge. At the school of Galileo, founded in Florence in the seventeenth century under the patronage of the Medici, the instrumental meteorology begins. This science elevates the study of atmospheric phenomena from merely qualitative to quantitative. The interest of Ferdinand II, Duke of Tuscany, for instrumental meteorology, laid the foundation for the subsequent quantitative and systematic study of atmospheric phenomena. The master glassmaker Moriani, built numerous thermometers each other identical, known universally as "small Florentine thermometers." Their distribution to Italian and foreign observers, gave a further impulse to the establishment of a synchronous meteorological observations service at international scale (Figure 1). At this early stage, the tasks of the observers were to conduct observations and measurements of some general air condition and temperature taken several times a day, but always at the same time. The assignment of observers went to religious since they were used to a very methodical way of life. Early observers arose in Florence, Vallombrosa, Cutignano, Bologna, Parma, Milan, Paris, Innsbruck, Osnabruck and Warsaw. Florence hosted the first historical data recorded: two very short ones, one from 26 November 1657 to 8 May 1658, the other from 12 February to 7 April 1658; a third one, that was much longer covered the period from 15 December 1654 to 31 March 1670 and is known as the Convent of St. Mary of the Angels series. Two years later the observers received also barometers, hygrometers and anemoscopes. Luigi Antinori, court chaplain, was coordinating survey operations from Florence. In addition to measuring instruments, Antinori provided to the observer the operating instructions and the forms to fill with the observations. The National Library of Florence keeps Galilean Manuscripts containing many of these forms

reporting the month and the year to which the report was done. The introduction of systematic objective observations instead of discontinuous subjective estimates, is in use until now, and it has represented for meteorology the key moment, the final break from all his previous methodological approach and the consequent recognition of the discipline as a real science [3-4].

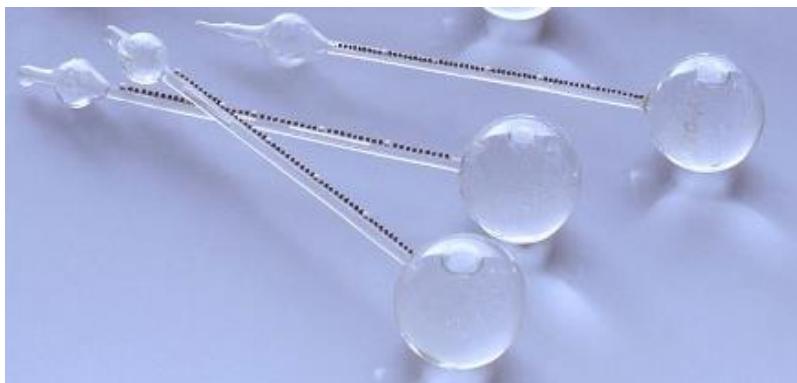


Figure 1. Thermometers designed by the Grand Duke Ferdinando II de 'Medici, the cinquantigradi thermometers were generally used to learn about the mutations of warm and cold air both outdoors and in closed rooms. The academics made wide use of this type of thermometers, which had the advantage of being comparable between them, especially for systematic meteorological observations.

2.2. Meteorology in 1800

From the beginning of XIX century, the atmosphere is investigated from a strictly physical point of view, according to the laws of mechanics and thermodynamics rising.

One of the first contributor was the French physicist Gaspard Gustave de Coriolis (1792-1843). In formulating the acceleration theorem of relative motion for mechanical systems in rotation, he introduced the concept of complementary acceleration and the corresponding force "apparent" that bears his name, force that is acting perpendicular to the motion, resulting in deviant effect on motion itself. Despite such composed force plays a fundamental role in the dynamics of the atmosphere, it should be pointed out that its author is not paid particular attention to the possibility of applying it in such a fluid. The American researcher William Ferrel did so, thus justifying the curvature of the air currents around the centres of high and low pressure and thanks to his studies on the general circulation of the atmosphere, meteorology fully entered into the domain of fluid dynamics. The period that saw very intense theoretical development, was the decade 1880-1890, with the physical and mathematical studies of German Hermann von Helmholtz. Starting from Euler form of the general equations of hydrodynamics, the scientist undertook an analytical study of the equilibrium conditions of the surface of separation between air masses. To explain the origin of the fronts and depressions, he

called into question the concept of hydrodynamic instability that will find its application in the theory of the polar front of the Norwegian Meteorological School. Von Helmholtz formalized the first law of thermodynamics in 1847, with the publication of a study on this subject. The discovery of the possibility of transforming the work into heat and vice versa, opened a new field of research: the study of the thermodynamic properties of the atmosphere. In parallel with developments of atmospheric physics, the nineteenth century saw significant progresses in statistical studies of the major climatic factors, primarily temperature and pressure, which was followed by studies in the fields of storms and cyclones. The American engineer William Redfield, was the first one to develop the theory of nature swirling and the direction of rotation of the winds in cyclones: counter clockwise in the Northern Hemisphere and clockwise in the Southern Hemisphere. The Redfield theory of cyclonic storms, was opposed by another theory based on the convection and the centripetal motion formulated by compatriot James Pollard Espy. Unlike Redfield who had preferred not to speculate explanations about the genesis of the cyclones, he hypothesized a strong upward motion at their centre, at minimum pressure, which consequently draws air from all directions. Pollard Espy was not fully knowledgeable on the effect of deflective force due to Earth's rotation while he had fully understood the role of water vapour in atmospheric thermodynamics [5-8]. For a long period this theory was the basis for the later theories formulated in convective cyclones both in America and in Europe. The study on the development of cyclones was deepened by both the German meteorologist Heinrich Wilhelm Dove and the English Admiral Robert Fitzroy. Both reached the conclusion that cyclones develop at the border between the polar currents, cold and dry, and the tropical currents, hot and humid and are that they are organized into families. Instead, only few studies have been done on anticyclones, perhaps related to the fact that they are normally accompanied by sunny and stable weather. In 1863, the Englishman Francis Galton discovers the particular characteristics of the anticyclone and the predominance of light winds at the centre, their clockwise rotation and the subsiding movement of the air column. Other than these two main types of pressure systems, the English meteorologist Ralph Abercromby will add another 5 secondary ones, namely:

- *Ridge*: high pressure area that, with isobars generally rounded or at an acute angle, and protruding from an anticyclone towards a low pressure zone;
- *Trough*: low-pressure corridor with isobars at an acute angle juts out from low pressure area;
- *Secondary cyclone*: low-pressure secondary centre;
- *Saddle*: the relative low-pressure area between two depressions and two anticyclones
- *Slope*: area characterized by pressure regularly decreasing and bounded by isobars almost straight and parallel.

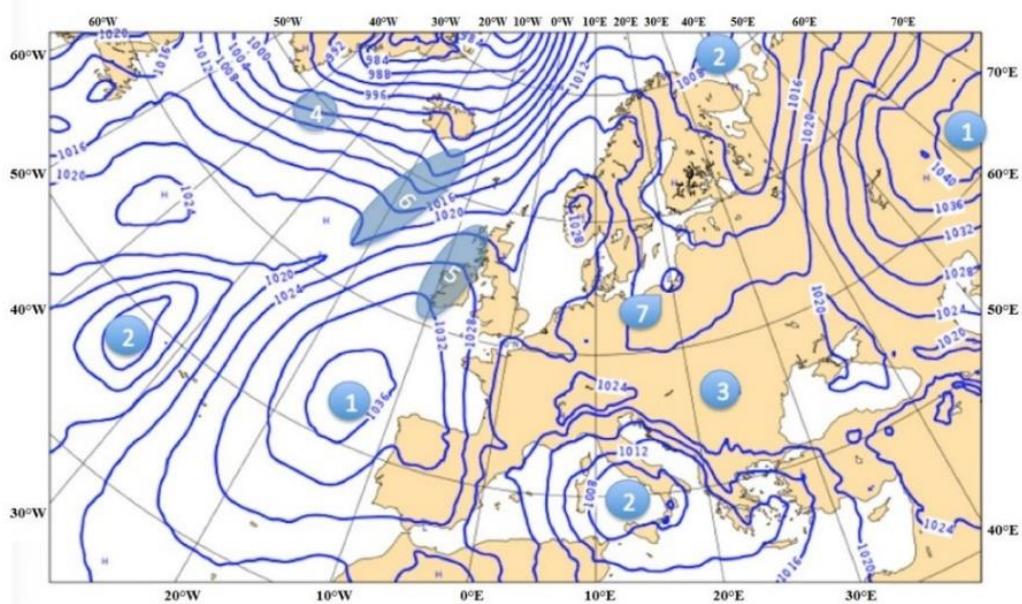


Figure 2. Pressure configurations: 1 Anticyclone; 2 Cyclone; 3 Saddle; 4 Slope; 5 Ridge; 6 Trough; 7 Secondary low.

Introduced by the author in his informational book “Weather,” published in 1888, this classification is, not only of historical interest, but it is still universally adopted (Figure 2).

2.3. Developments in Synoptic Meteorology

Antoine-Laurent de Lavoisier, father of modern chemistry, develops the concepts to represent the meteorological data, in particular the pressure, temperature, wind speed and direction observed synchronously, with great precision, on a geographical map, to forecast 24-48 hours in advance, the likely evolution. He thus laid the basis to the scientific development of a new meteorology: the synoptic meteorology. In October of 1790 he spells out the weather forecast rules based on the variations of the atmospheric pressure later published in the “Literary Magazine.” The scientist worked also to promote a campaign for the creation of a worldwide network of weather stations connected each other and operating in a strictly synchronous way. The worldwide network took over fifty years to be fully operational. The stations were connected each-other with the electric telegraph which allowed to quickly transmit the collected meteorological data and likewise send the weather safety alerts [9-11]. In the U.S.A., the physicist Joseph Henry implemented the weather communications with the telegraph in coordination with the Smithsonian Institution telegraphist proposing to open the daily communications with a

weather report like: “clear,” “rainy,” “windy” etc. instead of the usual “okay.” In 1843, the first weather maps were produced (Figure 3).

Further impulse to the development of modern meteorology occurred after the intense storm that affected the Black Sea on 14 November 1854. Both the British and French fleets that were supporting the Turkish fleet in the war between Russia and the Ottoman Empire (Crimean War) suffered serious damages. 38 between vessels and ships including the "Henry IV," the most prestigious of the British fleet sunk causing the death of about four hundred sailors. Less than a year after the storm, the French, under the guidance of the famous astronomer Jean Joseph Le Verrier, implemented the first meteorological network in the modern sense, made of twenty-four stations connected with the Astronomical Observatory of Paris (thirteen of which by telegraph). Le Verrier, studying the dynamics of the storm in light of atmospheric circulation known laws, was able to extrapolate the future evolution in a logical and rational way providing the first truly scientific approach to the complex issue of weather prediction. In 1873, during the Congress of Wien, participating nations agreed to set up an international organization in order to facilitate the exchange of weather information across national borders. Thus it was born the International Meteorological Organization (I.M.O).

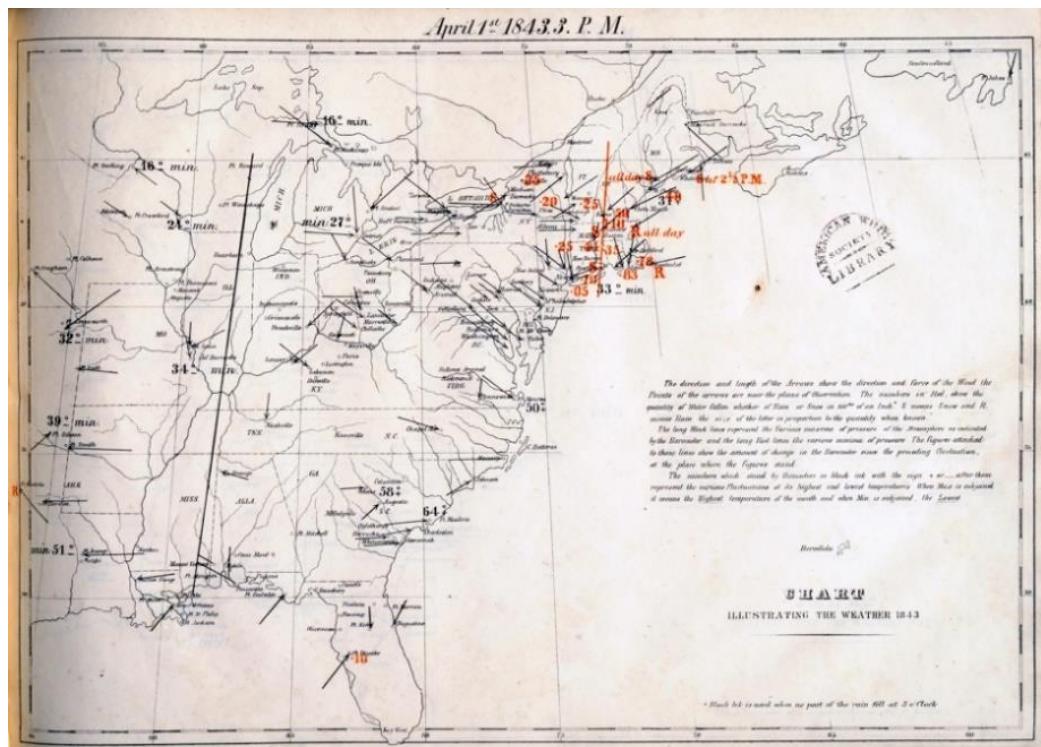


Figure 3. One of the first synoptic maps produced in 1843 from Espy's *Second Report on Meteorology* (source http://libweb5.princeton.edu/visual_materials/maps/websites/thematic-maps/quantitative/meteorology/meteorology.html).

3. HOW TO CREATE A MODERN METEOROLOGICAL MAP

What then has changed since the first synoptic maps? The modern system of meteorological observations, the fundamental and essential starting point for any meteorological activity, has today a multitude of systems unknown at the time of Le Verrier, that includes super-fast computers, satellites, data networks, electronic meteorological instruments, radar and more other tools (Figure 4).

One thing is, however, remained almost unchanged since the days of Le Verrier: the work of the almost 11.000 observation stations, that promptly make measurements of the main meteorological parameters such as atmospheric pressure, wind direction and speed, temperature, humidity, cloud coverage, on-going phenomena etc.

From their observations it is extrapolated a “snapshot” picture of the current state of the weather across the planet. This network of surface stations contributes significantly to the so-called Global Observing System (GOS) (Figure 5), one of the programs of the World Meteorological Organization (WMO), the specialized agency of the United Nations, created in 1950 and that is mainly involved in international cooperation and coordination in the field of meteorology, the state and behaviour of the atmosphere and its interactions with the oceans and soils and climate and weather that it produces [12].

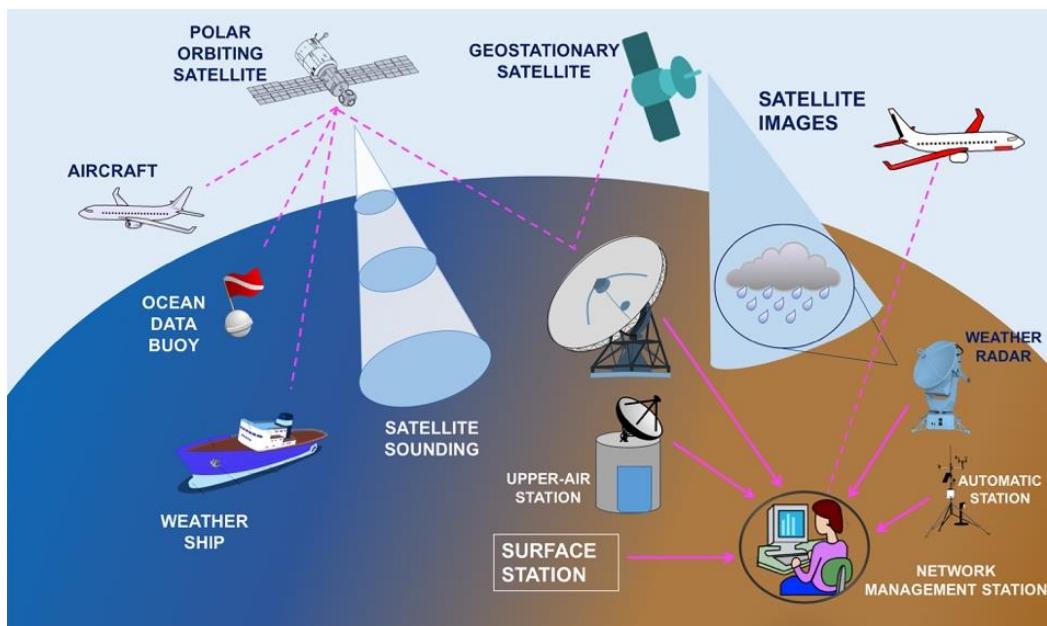
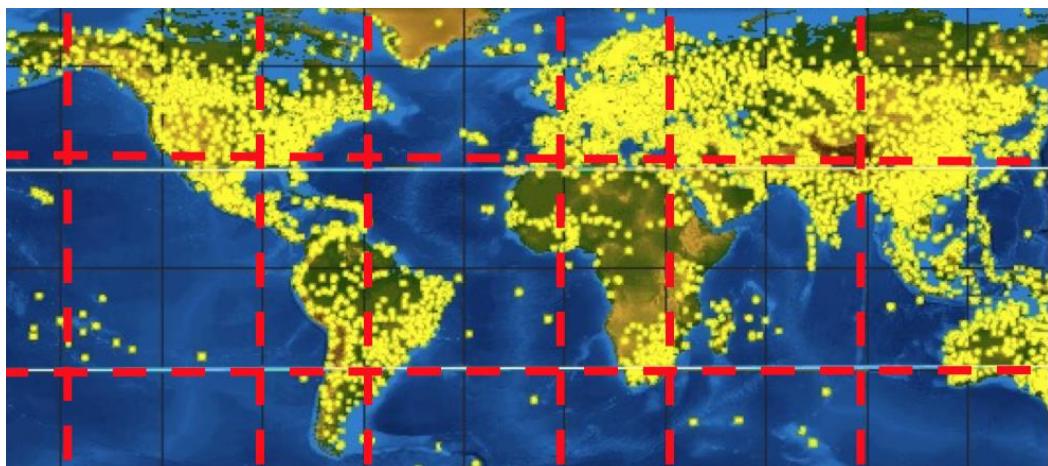


Figure 4. The Global Observing System.



Source: www.meted.ucar.edu.

Figure 5. The Global Surface Meteorological Station Network.

Parallel to the network of surface observation stations, which deal with collecting data in the lower atmosphere, there is a network of upper atmosphere observation stations, consisting of about 1300 stations, which at regular intervals of 6 or 12 hours release a balloons to make measurement of the main atmospheric parameters up to 30 kilometres of altitude. All data is collected by these networks and regularly exchanged data in real time. The exchange and circulation of meteorological data is done through another program of WMO: the Global Telecommunication System (G.T.S.). It is defined as: "The co-ordinated global system of telecommunication facilities and arrangements for the rapid collection, exchange and distribution of observations and processed information within the framework of the World Weather Watch."

4. OVERVIEW OF WEATHER MAPS AND SYMBOLS: OBSERVATION AND MESSAGES

Each weather station, whether fully automated or with observer staff, must make the meteorological measurements, translate them into a standard meteorological code or message, store them on a suitable base (paper until a few years ago, computer nowadays) and transmit this message on G.T.S. so that it is available in real time all over the world. For the automatic stations the whole process is almost instantaneous and managed entirely by electronics, while for the stations with personnel it takes place substantially without any significant differences compared to a century ago.

About 10 minutes before the observation time, the observer reads the instrument, taking the data of temperature, air humidity, direction and strength of the wind, pressure

etc. He also execute subjective observations such as the quantification of the type, height and the amount of clouds covering the sky in the vicinity of the point of observation, the horizontal visibility and any other visible meteorological phenomena.

sky cover	wind	selected weather symbols	fronts and radar
○ clear	○ calm	* rain	cold front 
① 1/8	— 1-2 knots (1-2 mph)	▽ rain shower	warm front 
● scattered	— 3-7 knots (3-8 mph)	[] thunderstorm	stationarity front 
◐ 3/8	— 8-12 knots (9-14 mph)	? drizzle	occluded front 
◑ 4/8	— 13-17 knots (15-20 mph)	* snow	high pressure system 
◑ 5/8	— 18-22 knots (21-25 mph)	▽ snow shower	low pressure system 
● broken	— 23-27 knots (26-31 mph)	○ freezing rain	
◐ 7/8	— 48-52 knots (55-60 mph)	○ freezing drizzle	
● overcast	— 73-77 knots (84-89 mph)	— fog	
⊗ obscured	— 103-107 knots (119-123 mph)	∞ haze	
Note Multiple rain or snow symbols indicate storm intensity: light (2 symbols) moderate (3 symbols) heavy (4 symbols)		— smoke	
		↑ \$ dust or sand	
		→ + blowing snow	

Figure 6. Meteorological Symbols used worldwide.

The next step, until a few decades ago, included the completion of the so-called “station’s book” on which were annotate all measures taken to the instruments. Today, the raw data are inserted on special software that provide the code according to the

standards in use. The meteorological code universally adopted is called “SYNOP” and contain in summary form all the data that allow any meteorologist to know exactly the weather observed at any locations of the Earth. The SYNOP message is a numeric code composed by groups of five numbers arranged in such a manner that each group of the code is uniquely a data type. For example, the following code:

“SMIY01 111800 16429 11462 73504 10044 20021 30009 40021 55005 60232
72196 85360 333 20040 32 // 55005 55300 82915 83818 85356 2 // /”

is the SYNOP message of Sigonella station on day 11 of the current month at 1800 UTC. Each group of the code has a codified meaning. In the example the wind was from 350° 4 knots, the temperature of 4.4°C and so on. For further information, please refer to dedicated publications. SYNOP is a specific message for synoptic meteorology and is produced simultaneously from all the stations around the world with a time step of 3 hours beginning from 00 UTC.

In order to plot the synoptic observations on a map, it was at least necessary to take a number of forms, capable of translate the observed data in graphical symbols (Figure 6).

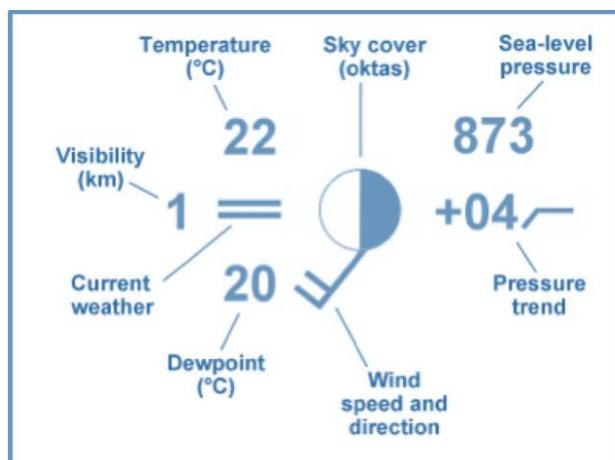


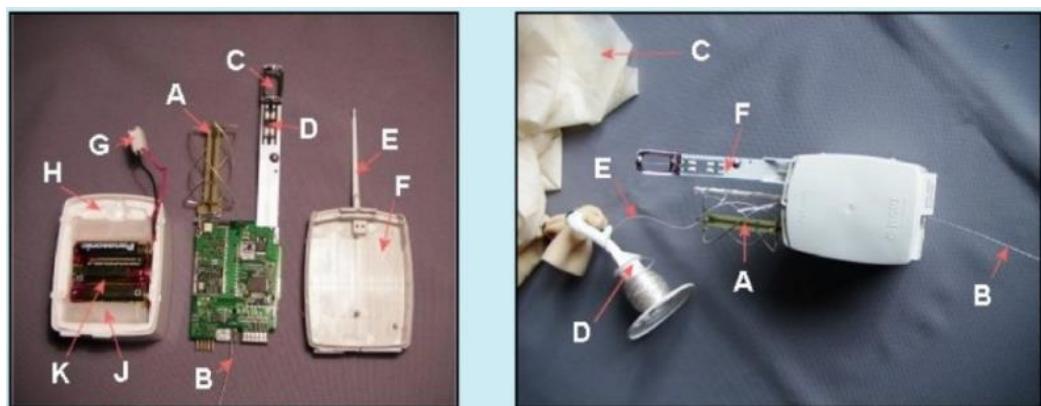
Figure 7. Station Plot.

The result of this process, called “station plot,” produce a group of symbols and numbers that can synthesize the whole process of observation, (Figure 7).

In addition to SYNOP, which is the most widespread exchange format of weather data, there are also other types of codes, which are used especially in aviation. It is the case of “METAR” message, an aeronautical meteorological code used for the observation performed by aerodrome meteorological stations. Characteristic of the METAR message is the speed of preparation and dissemination. In this message, the measured data are rounded to the closest unity. It is also an alphanumeric code, more clear than SYNOP, which contains the main meteorological information useful for aircraft pilots.

“METAR LICC 182200Z 35008KT 9999 RA SCT020 BKN035 OVC090 12/10 Q1010” is for example the Metar of Catania aerodrome.

As for the surface observation stations, the stations that measure the upper atmosphere data start the observational activities before the time of observation. Moreover, they have the delicate task of preparing the necessary instruments to collect data, called radiosondes. They consist of small boxes of polystyrene, which enclose internally all the sensors for measurement of temperature, pressure and humidity in addition to the electronics for the transmission of data to the ground station (Figure 8).



- A: GPS receiver antenna
- B: Transmitter antenna
- C: Temperature sensor
- D: Humidity sensor
- E: Hooking of the cord
- F: Box
- G: Power connector
- H: Box
- J: Mass compensator
- K: Battery pack

- A: GPS receiver antenna
- B: Transmitter antenna
- C: Balloon
- D: Sprocket of twine
- E: Twine
- F: Temperature and humidity sensors

Figure 8. Radiosonde.

Such equipment, attached to a balloon inflated with helium and released simultaneously from all the upper observation stations of the world at 00 and 12 UTC, send temperature, humidity and pressure data, in addition to the wind calculated by GPS, to the receiving station (Figure 9).

After the bursting of the balloon, which normally occurs between 20 and 30 km above sea level, and in any case after one hour from the time of launch, the transmitted data are encoded in a message called “TEMP” and forwarded to the appropriate Communication Centre through the G.T.S. network.



Figure 9. Release of balloon at midnight at Mario Zucchelli Station the Italian Base in Antarctica.

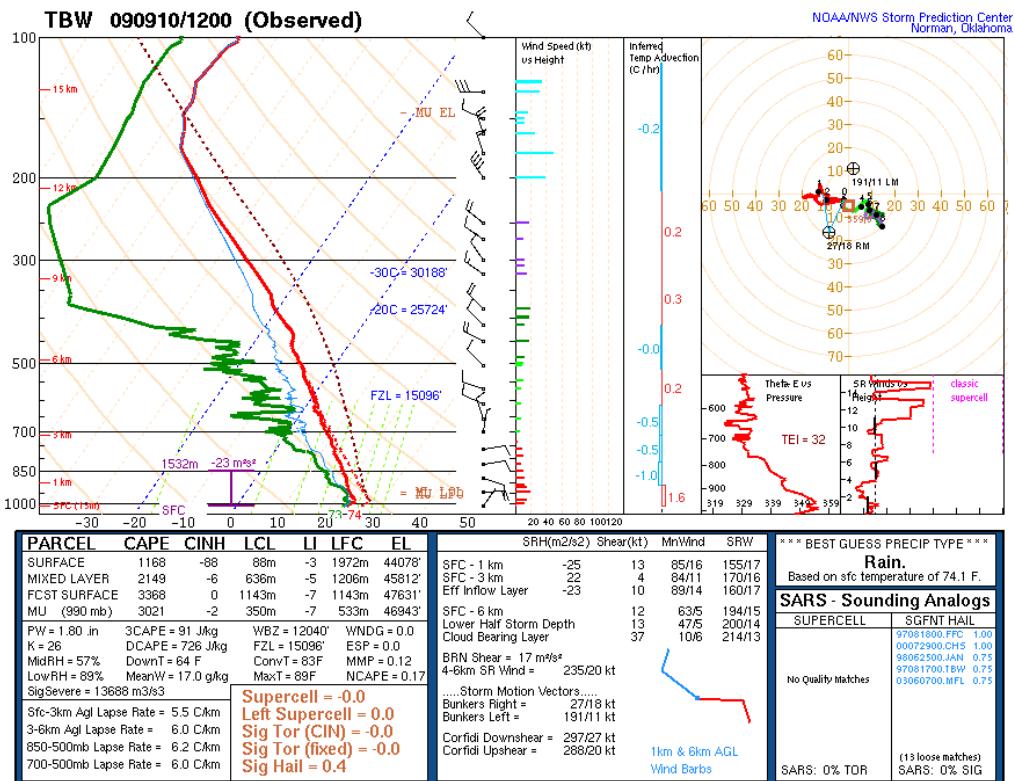


Figure 10. Thermodynamics diagram and data received from radiosonde.

The messages TEMP, in addition to the station identification and the date-time groups, contain data of temperature, humidity and wind to the various pressure altitudes touched by the radiosonde. These data can be plotted on maps or analysed by atmospheric thermodynamic diagrams, which summarize the characteristics of the column of atmosphere crossed by the radiosonde (Figure 10).

5. SURFACE AND UPPER ANALYSIS MAPS

The enormous amount of data that, through the G.T.S., regularly flow into the main Meteorological Centers around the world, represent the raw material to start the production of any kind of maps. The first step, which will get to the final release of the weather map, is the plot of the graphic symbols - station plot - on a map, in correspondence with the geographical location it's clear, however, due to the excessive crowding of data, that this type of representation does not lend itself to be used for any kind of analysis [13-14]. The next step will therefore be to draw the isolines, using the measured data to the stations, on a map cleaned thinning out most of stations plot and leaving only the most significant (Figure 11).

Similarly, it is possible to draw contour lines of the main data observed: isobars for pressure, isotherms for temperature and so on. The final result will be a map that contains one or more fields, represented by contour lines, easy to read and interpret (Figures 12 and 13).

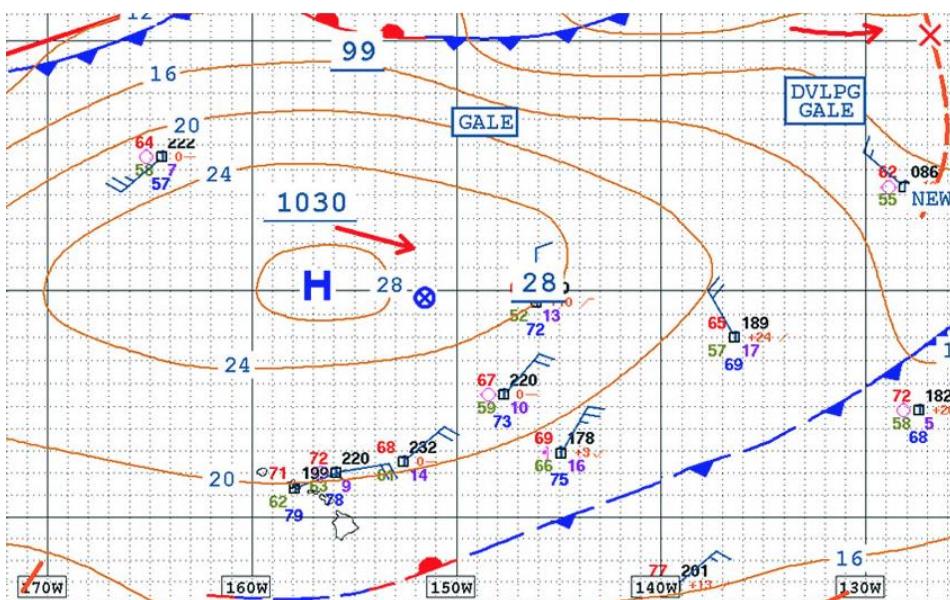


Figure 11. Map of analysis containing the pressure field to the ground, represented by isobars (yellow lines), in which have been left only some station plot.

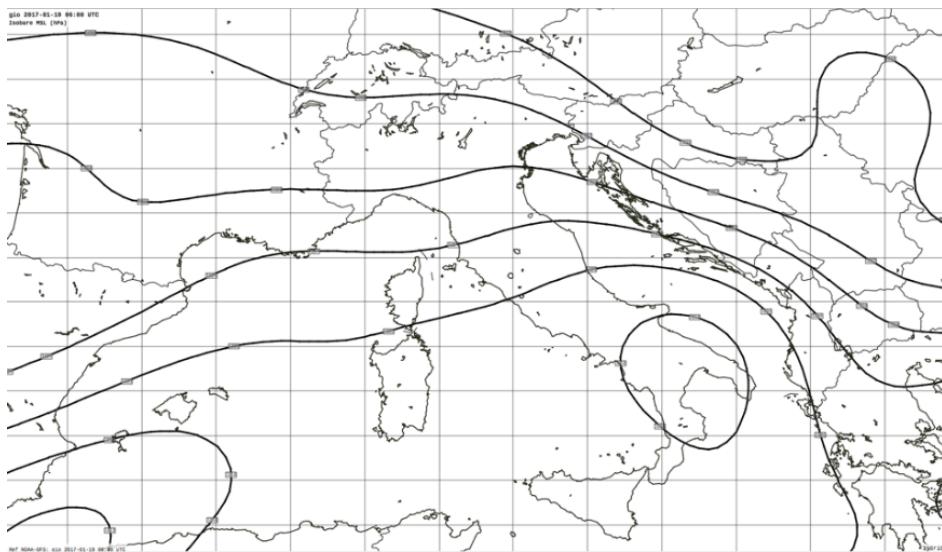


Figure 12. Plot of surface pressure field (ZyGrib freeware).

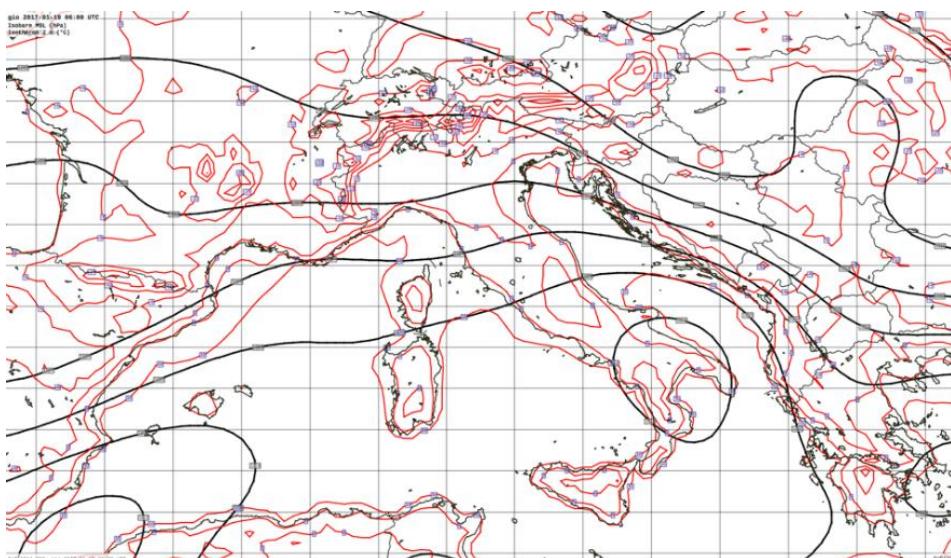
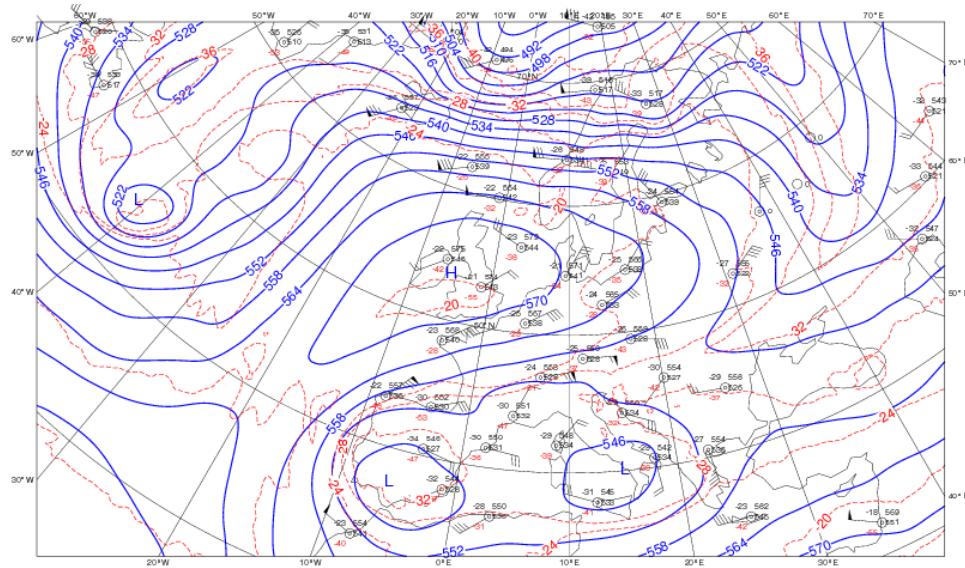


Figure 13. Plot of surface temperature and pressure fields (ZyGrib freeware).

The process of production of maps at high altitude does not differ much from the one to the ground: in place of the surface pressure, the height of the isobaric surfaces are represented. For this reason, the upper maps are also called absolute topographies and altitudes are expressed in geopotential heights, a term that is obtained from the relationship between geopotential (the work necessary to overcome the force of gravity and move upwards, to a certain height), a unit mass of air, and gravity at sea level (Figure 14).



are thus diverted, in their initial momentum, to the right in our hemisphere and to the left in the southern hemisphere.

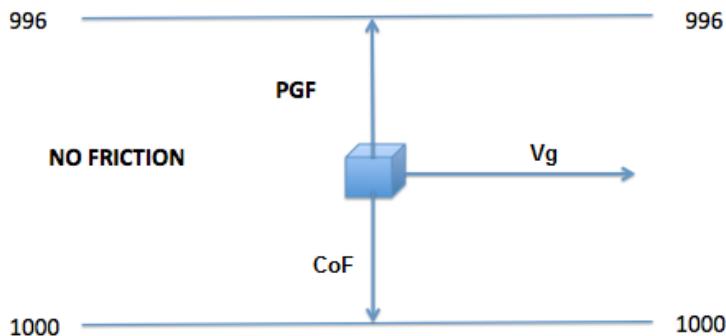


Figure 15. Wind resulting from the balance between the Coriolis force and the pressure gradient force.

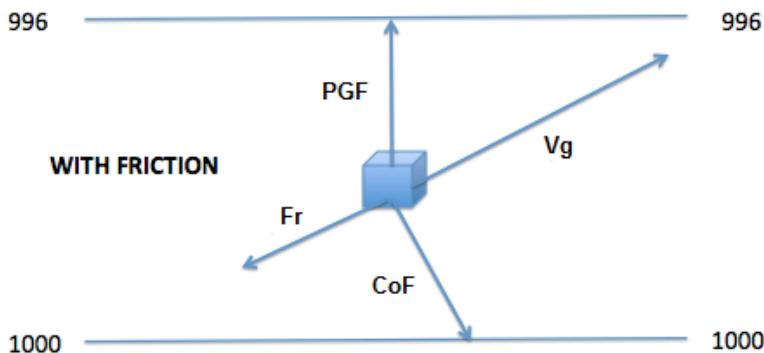


Figure 16. Wind resultant from the balance between Coriolis force, pressure gradient force and friction.

Therefore, in the hypothetical case of straight and parallel isobars and ignoring for the moment all forms of friction, the wind resulting from the balance between the Coriolis force and pressure-gradient force, will give rise to what we call geostrophic wind V_g , as shown in Figure 15.

The geostrophic wind will therefore be parallel to the isobars. However, an air mass moving on a surface such as that of the Earth, will be subject to the resistances of friction F_r that depend upon the roughness of the surface and which act in the opposite direction to the motion. Introducing this force, the new equilibrium will be as follows in Figure 16.

The resultant of this new balance will be a wind (a-geostrophic), which will cut the isobars pointing toward the low pressure, with an angle that will be greater the greater the friction. On the sea or over a very smooth land surfaces this angle is between 10 and 30 degrees, while on rough land or mountain areas you can get to even exceed 60-70 degrees. These considerations help us to understand that the surface wind forecast will follow the isobars, converging, with an angle comprised between 10 and 70 or more degrees, towards the low pressure [15]. Furthermore, the same considerations allow us to establish that in the case of closed circulations of high or low pressure, winds will assume

a counterclockwise rotation (or cyclonic) around the low-pressure centers, and clockwise (or anti-cyclonic) around high-pressure centers. For the considerations made on the friction they will tend to diverge from the high pressures and to converge toward the low.

The convergence that occurs around low-pressure centers, is one of the mechanisms which produces the lifting of the air masses.

When the mass of moist air that converges around low-pressure centers begin the lifting process, it expands and cools, condensing the water vapor that contains and giving rise to the typical cloudiness of the low pressure zones. Conversely, the divergence produced by the high pressure center that draws air from the top down dimension is compressed and heated, favoring the dissipation of any present clouds (Figure 17).

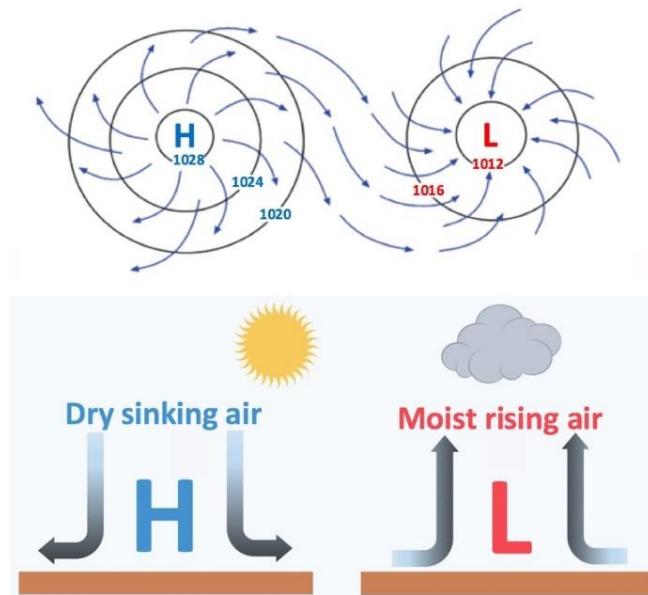


Figure 17. Motion of air around a High and a Low pressure in Northern hemisphere.

7. FROM SYNOPTIC METEOROLOGY TO CLIMATE ANALYSIS

The huge amount of data, continuously observed and archived by weather stations around the world, is one of the most important resources for the development of new branches of meteorology such as the statistical meteorology and climatology. After the invention of the first measuring instruments, one of the key issues was what to do and how to use the data series collected. The first analysis carried out using meteorological data, were simple descriptive statistics, or study about the variability of a phenomenon since the data were collected. This led to the first attempts to classify climates of different places, depending on the temperature and average rainfall occurring during the year.

In 1817 Alexander von Humboldt drew annual-mean temperatures on a world map. Wladimir Koeppen (1846-1940) refined this map and plotted seasonal temperature range in 1884, leading to his climate classification. This classification followed that of plants realized by Linnaeus in 1735, being likewise hierarchical, with major categories subdivided, and then subcategories divided again, and so on. In fact, Koeppen had initially studied botany at St Petersburg, later completing a Ph.D. at Heidelberg on the effect of temperature on plant growth. At the highest level his system is based on five sets of temperature limits. These were developed from his categorization in 1884 of thermal zones suited to various kinds of vegetation (Figure 18).

In 1924 Koeppen became associated at Gradz University with Rudolf Geiger (1894-1981) and collaborated with him in producing the 1936 system of climate classification. Geiger established the discipline of microclimatology as he collected a wealth of observations to understand ‘the climate near the ground’ (to quote the title of his book, translated into English in 1960), and its variations due to topography and land use [16-18].

In the USA, Warren Thornthwaite (1892-1963) developed a hierarchical classification in 1931, essentially in terms of the annual pattern of soil-moisture conditions. These were regarded as depending in a complicated manner on the monthly input as rain, and implicitly on the output as evaporation, indicated by temperature.

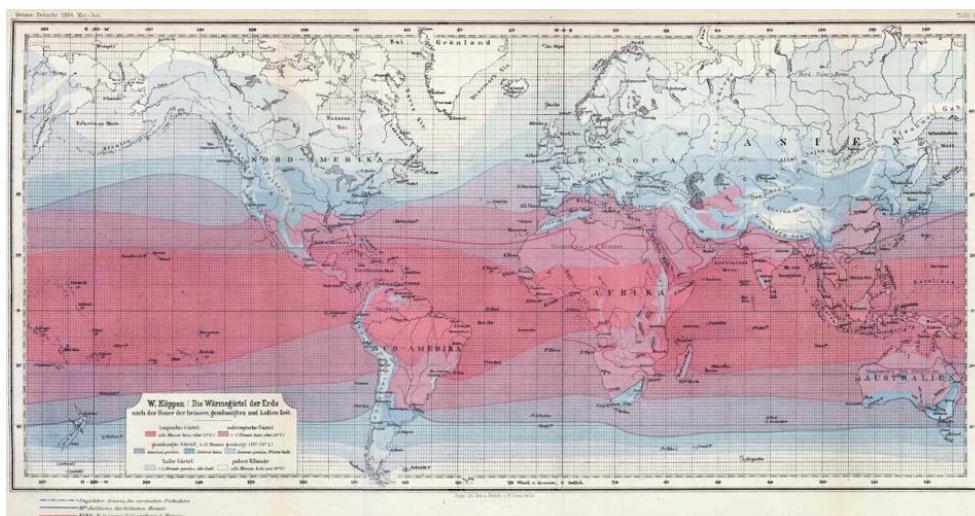


Figure 18. The first Koeppen Climate classification map.

This kind of maps are useful to represent the extreme environments and to explain the effects that make such environment so extreme.

As an example we take into account the Atacama Desert (Chile, USA) that is the most arid place on Earth, where every year falls, on average, no more than 0.08 mm of rain. Its geographical position plays a key role in explaining this negative record. The

area is protected by moisture on both sides, with the Andes Cordillera to the East and the coastal mountains to the west. On the desert eastern mountainside, where the peaks reach to over 5000 meters, the Andes Cordillera is a real barrier to the flows coming from the East. The katabatic winds that affect the area are very dry and contribute to heat the air for adiabatic compression (see Figure 19).

These environments are characterized by high aridity, very hot and low temperatures, high salinity and high values of pH and by the fact that many living organisms, the extremophiles, can survive in these conditions thanks to the synthesizing of the trehalose, a disaccharide that is revealed to be a cryptobiotic-activating substances [19-31].

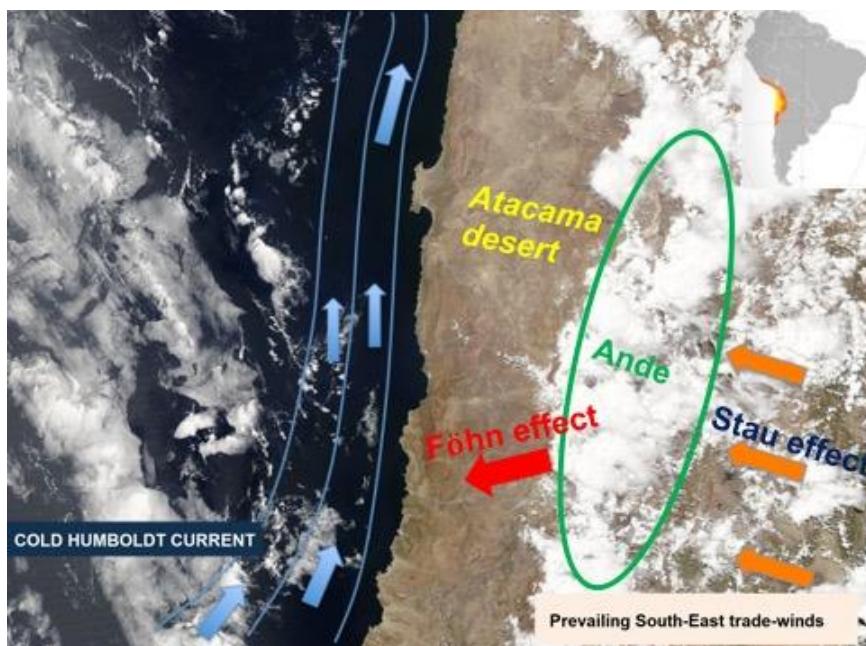


Figure 19. Atacama Desert.

Concerning the extremophile present in the Atacama Desert, it is possible find the plant of resurrection, i.e., *Selaginella lepidophylla* [39-55]. Such a plant that synthesizes trehalose is able to adapt itself at the conditions of prolonged drought in this environment [56-69]. Furthermore, it also lives for 50 years against numerous total dehydration processes without damaging it, and after a process of rehydration, it regenerates [70-81]. This disaccharide is object of many studies with different techniques [82-93].

In parallel to these studies of climate descriptions based primarily on statistical considerations, new techniques of analysis of the time series were developed. The Fourier analysis applied to a time series $\alpha(t)$ is a technique that allows the study of the signal α in the frequency domain, due to the decomposition of the temporal function itself in an infinite number of harmonics (fundamental waves), in which the 'amplitude of each

harmonic represents the weight that it has in the original signal [94-102]. The decomposition into harmonics is expressed by the inverse Fourier function, defined as

$$\alpha(t) = \frac{1}{2} \int_{-\infty}^{+\infty} A(\omega) e^{i\omega t} d\omega \quad (1)$$

where the inverse relationship, the Fourier transform, it is defined as:

$$A(\omega) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \alpha(t) e^{-i\omega t} dt \quad (2)$$

with i imaginary unit, ω angular frequency of the harmonic (rad/s), given $\omega = 2\pi/T$ and T period of harmonica in seconds. The analysis in the frequency domain is conducted to highlight certain properties not immediately recognizable in the time representation of a signal. The spectral analysis of climate data is now a widely used technique in the world, and through it many dark sides and little known of the Earth's climate system, were revealed [103-109].

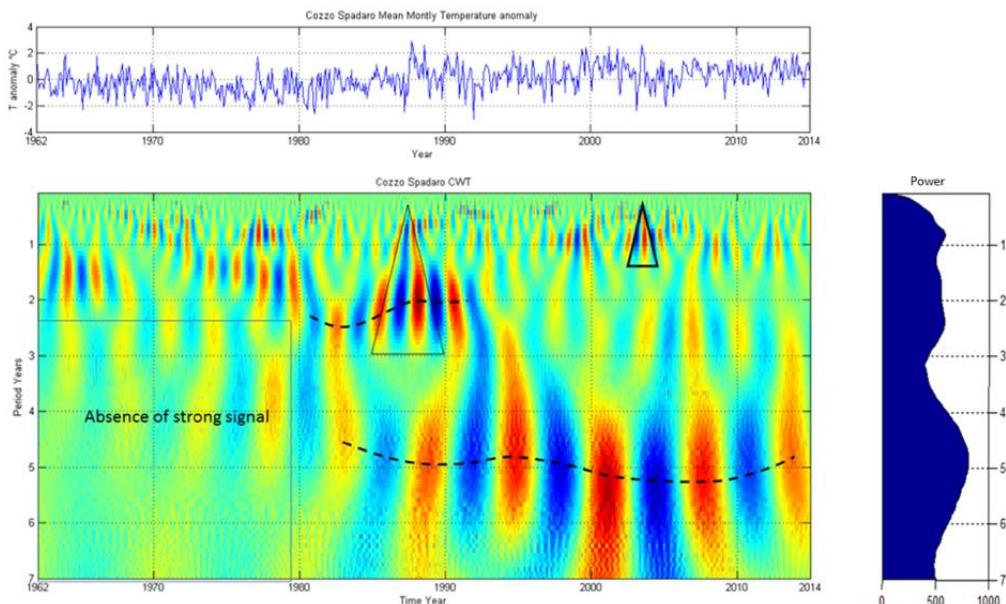


Figure 20. Example of wavelet analysis on a temperature time series.

Thanks to analysis on paleo climatic data was possible, for example, reconstruct and correlate the duration of the astronomical cycles with terrestrial glaciations. Further developments, which benefited Meteorology and Climatology, came undoubtedly from the use of wavelet analysis. The Wavelet analysis is a powerful mathematical tool capable of providing a representation time-frequency of any signal analyzed in the time domain [110-119]. They can be used to analyze time series that contain nonstationary

power at many different frequencies. In the case of meteorological and climatological series this type of analysis is particularly appreciated being able to extract valuable information from the signal. Compared for example to the simple Fourier transform, wavelets allow to find not only in the value of certain frequencies present in a non-stationary series, but also to identify the time interval in which these frequencies have been present and predominant. These sophisticated tools have been used in several studies of climatology and the scientific literature is rich of many examples [120-127]. The continuous wavelet transform of a discrete sequence x_n with a scaled and translated version of $\psi_0(\eta)$:

$$W_n(s) = \sum_{n'=0}^{N-1} x_{n'} \psi * \left[\frac{(n'-n)\delta t}{s} \right] \quad (3)$$

where the (*) indicates the complex conjugate. By varying the wavelet scale s and translating along the localized time index n , one can construct a picture showing both the amplitude of any features versus the scale and how this amplitude varies with time as reported in Figure 20.

CONCLUSION

In this paper, after a brief history of meteorology during XVIII, XIX and XX centuries, it has been described the evolution of the meteorology as consequence of the evolution of the instruments to measure the main characteristics of the atmosphere such as temperature, pressure and humidity. The invention of the telegraph gave a further strong impetus to the development of modern meteorology and made possible the exchange of the observed data. After the II Word War, the establishment of the World Meteorological Organization (WMO) in March 1950, following the entry into force of its Convention, and the designation of WMO in 1951 as a specialized agency of the United Nations, announced a new era for international cooperation in the field of meteorology, hydrology and related geophysical sciences. Meteorology has had a further impulse thanks to the diffusion of personal computers and the Internet, which have enabled millions of people to be able to consult maps and products previously available only in large computer centers. This possibility of having meteorological products has not been followed by a necessary training and education of users, who often cannot correctly decipher the contents of the meteorological maps available online. The aim of this paper is to help students that approach to meteorology to understand the origin and the evolution of the Science of the Atmosphere and to be able to read and interpret correctly the information contained in the meteorological maps.

ACKNOWLEDGMENTS

The authors wish to thank the Italian Air Force – Meteorological Service for map of geopotential height and temperature in Figure 14.

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Chapter 10

FOURIER AND WAVELET ANALYSES OF CLIMATE DATA

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ABSTRACT

In this paper, we report a case study, addressed to scientific curricula graduate students, concerning the application of Fourier Transform (FT) and Wavelet Transform (WT) on climate data and on their connections with Milankovitch’s cycles. It is shown how, contrarily to FT that furnishes only the signal frequency values, WT allows to get information on the time evolution of the frequencies content. From the performed FT and WT analyses the presence of glacial maxima with time intervals of around 100000 years emerges. These have been connected with the variation of the eccentricity of the Earth’s orbit. Moreover, between 1.8 and 1.3 million years ago, glacial maxima repeat about every 41.000 years in agreement with the cycle of variation of the Earth’s axis inclination.

Keywords: wavelet transform, Fourier transform, climate

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INTRODUCTION

Signal analysis has become increasingly important in many University curricula also due to the increase in computational efficiency [1-8]. In this framework Fourier Transform (FT) and Wavelet Transform (WT) are extensively applied to detect signal periodicities. Following Fourier, a periodic function $f(t)$ can be expressed as [9-14]:

$$f(t) = \sum_{n=0}^{\infty} [P_n \cos(n\omega t) + Q_n \sin(n\omega t)] \quad (1)$$

where P_n and Q_n are the Fourier coefficients, where it is:

$$P_n = \frac{2}{T} \int_0^T f(t) \cos(n\omega t) dt; \quad (2)$$

and

$$Q_n = \frac{2}{T} \int_0^T f(t) \sin(n\omega t) dt. \quad (3)$$

P_n and Q_n are called the $f(t)$ harmonic components.

Furthermore for not periodic functions, one can introduce the Fourier transform:

$$\int_{-\infty}^{+\infty} f(t) e^{i\omega t} dt. \quad (4)$$

When it is necessary to highlight the signal frequency localization one can take advantage from the use of WT. In particular, WT associates to a $f(t)$ function, another function $WT(scale, \tau)$, where $scale$ is a positive parameter and τ represents a time shift [15-21]. So WT decomposes $f(t)$ into wavelets components $\frac{1}{\sqrt{scale}} \psi\left(\frac{t-\tau}{scale}\right)$, as it follows:

$$WT(scale, \tau) = \frac{1}{\sqrt{scale}} \int_{-\infty}^{+\infty} f(t) \psi^*\left(\frac{t-\tau}{scale}\right) dt \quad (5)$$

ψ^* is the ψ conjugate complex.

It should be noticed that, differently from FT which simultaneously shows signal frequencies, WT shows at what time they are [22-25].

THE CLIMATE GEOSYSTEM

It is well known that at any point on the Earth's surface, the energy from the Sun changes during the day and year but also according to longer cycles that depend on Earth's movements within the Solar System. This cyclical variation of solar energy

coming to Earth, known as solar forcing, causes changes in the surface of our planet: temperatures rise during the day and lower during the night, increase in summer and decrease in winter. The term climate refers to the average state of the atmosphere in a particular location in the Earth, as it results from observations over a long time period (at least thirty years), and the variations of these atmospheric conditions during the solar forcing cycles. The climate is described by the average values of the seasonal weather conditions observed in the vicinity of the Earth surface (surface air temperature), the humidity of the air, the cloud cover, the amount of precipitation, the wind speed and of other weather conditions [26-28].

A comprehensive description of climate includes, in addition to these common weather statistics, some non-atmospheric features of the Earth's surface environment, such as soil moisture, continental water outflow, ocean surface water temperatures and speed of marine currents.

Geological evidence shows that, in the past, several periods of global warming and periods of glacial cold have been alternating. These alternations are very irregular since substantial changes in the climate may occur in a few decades or evolve slowly over many millions of years.

Some climatic variations can be attributed to external factors, such as fluctuations in the amount of solar radiation; others can be attributed to changes that occur within the same climate system. Both these variations, related to external or internal causes, may amplify or be damped by feedback processes.

The glacial cycles of the Pleistocene era that occurred around 1.8 million years ago are among the most spectacular recorded climatic variations. A glacial cycle begins with a gradual diminution in temperature of about 6 - 8°C, leading from a warm interglacial age to cold glacial ice age. With climate cooling, the amount of sea ice increases and during the winter on the emerged lands falls a greater amount of snow than that which fuses during the summer. In this way the volume of polar caps and the area occupied by them increase, while the volume of ocean water decreases. With the expansion of glacial masses to smaller latitudes, the amount of energy reflected in space is greater and, consequently, the air temperature decreases further. This represents an example of positive feedback due to the increase in albedo. In addition, the sea level is lowered and this causes the emergence of continental submerged portions. During the glacial age, at the glacial maximum, large and powerful glaciers, cover large areas of the emerged lands. The glacial age ends with a rise in temperature when, with the retreat of glaciers (continental and mountain), the water is transferred from the cryosphere and the sea level rises [28-32].

These climate condition oscillations may give rise, with a given periodicity, to extreme environments characterized by harsh conditions which are accessible only to organisms, the extremophiles, that can survive thanks to different survival strategies [33-

49]. The study of these environments as well as of the survival mechanisms are of great interest due to their important applicative fall out [50-61].

In this framework it is useful to mention that at the Vostok scientific station, in the icy Antarctica, a group of Russian and French scientists has been working for decades to try and rebuild the Earth's climate story. In the 70's and 80's of the twentieth century, scientists at this station punctured the East Antarctic ice to a depth of 2000 m and took a series of "carrots" to be subjected to detailed laboratory studies. These carrots have a stratification produced by annual cycles of snow transformation into ice. A careful count of the layers, from the top down, made it possible to define the age of the ice.

On trapped air, in small bubbles, measurements of isotopic oxygen ratios and gas composition were carried out in the different layers of ice. Based on these stratigraphic evidence, researchers have rebuilt a detailed history of glacial cycles during the last 160,000 years. In 1998 the drilling performed at Vostok had reached the depth of 3,600 m, penetrating the ice accumulated during the last glacial cycles and so climatic recordings have been extended to more than 400,000 years ago.

The obtained data corroborate the hypothesis that Earth's millenary movements - according to Milankovitch's cycles - control the alternation of glacial and interglacial ages. They have also shown that air temperatures are also related to greenhouse gas concentrations in the atmosphere. The results obtained with Vostok's studies were confirmed by those obtained for other ice caps, both in Antarctica and in Greenland.

These findings have not been easily achieved. The Vostok station, located in the central part of East Antarctica at an altitude of about 3500m, is an inhospitable place to conduct research. Its average annual temperature is - 55°C and the lowest reliable temperature was - 89.2°C, recorded in 1983. Scientists need not only endure these extreme conditions, but they also need to be careful not to cause fusion or the contamination of ice during carottage, during the transport of samples to the analysis laboratories and during their conversion. They must also be able to exclude results that may be misleading, such as those arising from carbon dioxide reactions with impurities contained in the ice.

More in detail, the measurement of the abundance of oxygen isotopes, preserved in marine sediments and glacial ice, provides accurate evidence of variations in temperature during the Pleistocene. Pleistocene marine sediments contain many fossils of foraminifers: small unicellular marine organisms that secrete calcite shells (CaCO_3). The amount by which the various isotopes of oxygen are incorporated into these shells depends on the isotopic ratio of seawater in which these organisms lived [62-68].

The water (H_2O) containing oxygen-16, O^{16} , the lightest and most common isotope of oxygen, evaporates more easily than the water that contains the heavier-oxygen 18, O^{18} .

As a consequence, during the glacial age the oxygen-18/oxygen-16 ratio of ocean water increases whereas in the ice layers diminishes. In fact, water containing oxygen-16 evaporates from sea and then is trapped in the ice of glaciers, while oxygen-18-rich water

remains preferentially in the oceans. By measuring the oxygen-18/oxygen-16 isotopic ratio in layers of marine sediments, it is possible to obtain information on the surface water temperatures and on the volume of ice. Figure 1 reports δO^{18} and temperature variation as a function of time during the last 5.5 M years [69-71].

Furthermore the examination of the gas trapped in the ice can furnish information on the atmosphere, including the concentration of carbon dioxide and methane CH_4 .

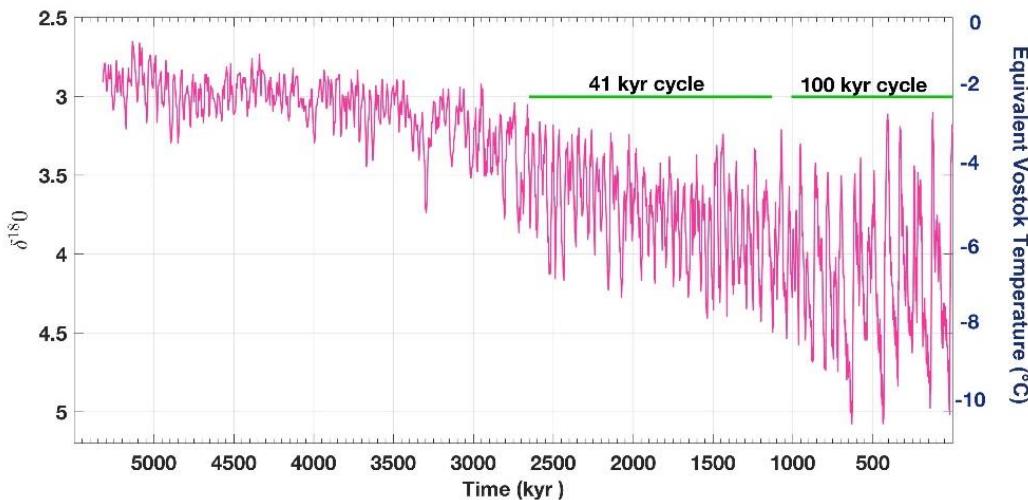


Figure 1. δO^{18} and temperature variation as a function of time during the last 5.5 M years.

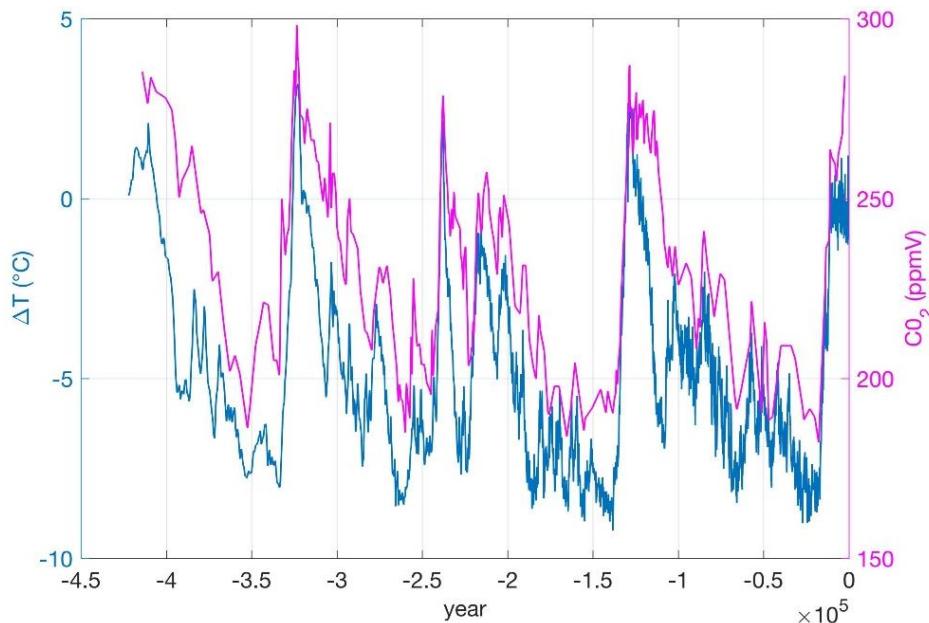


Figure 2. Some data obtained at the Vostok station in the East Antarctica. In such a case positive peaks show high temperature and carbon dioxide concentrations.

Figure 2 shows the trend of atmospheric temperatures and concentrations of two important greenhouse gases, carbon dioxide and methane CH₄, rebuilt according to data provided by the famous ice drilling carried out at Vostok station in East Antarctica [72-76]. A modification of the *solar forcing* can be a plausible answer to these climate fluctuations. As a matter of fact, these variations can be related to Milankovitch's cycles, i.d. with long-term periodic motions (millenary motions) of Earth, so called by the Serbian geo-physical name Milankovitch.

More in details, Milankovitch's cycles, that can be related to global climate variations, are of three types:

- (i) A first cycle concerns the orbit of the Earth around the Sun. Its elliptical shape varies periodically, in millennia, becoming more and less “crushed”. The variation of the shape of the orbit can be expressed by its eccentricity: the value of eccentricity is very small in an almost circular orbit and grows as the orbit becomes more and more elliptical. Depending on the orbit's eccentricity, the average amount of solar radiation received from Earth changes. In Figure 3 the variation in the eccentricity of the Earth orbit, which has a cycle of about 100,000 years, is shown; during this cycle the value of the eccentricity passes from the maximum to the minimum and again reaches the maximum [77-83].
- (ii) A second astronomical cycle affecting the distribution of solar energy received by Earth is the change in the inclination of the Earth's axis: the angle between the Earth's rotation axis and the normal plane of the orbit (which is now $23^\circ 27'$) does not remain constant over time, but varies from a minimum of $21^\circ 55'$ to a maximum of $24^\circ 20'$, with an average time of approximately 41,000 years (see Figure 4).
- (iii) A third astronomical cycle is connected with the Earth's axis which performs a double-conic motion, called solar-precession, with a period of about 23,000 years, as reported in Figure 5. This movement also changes the amount of heat the Earth receives from the Sun at different times of the year, albeit has a lesser extent than the other two cycles.

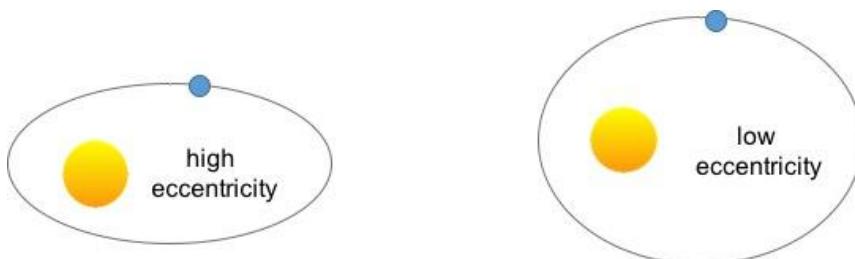


Figure 3. Orbit eccentricity. The variation in the eccentricity of the Earth orbit has a cycle of about 100,000 years.

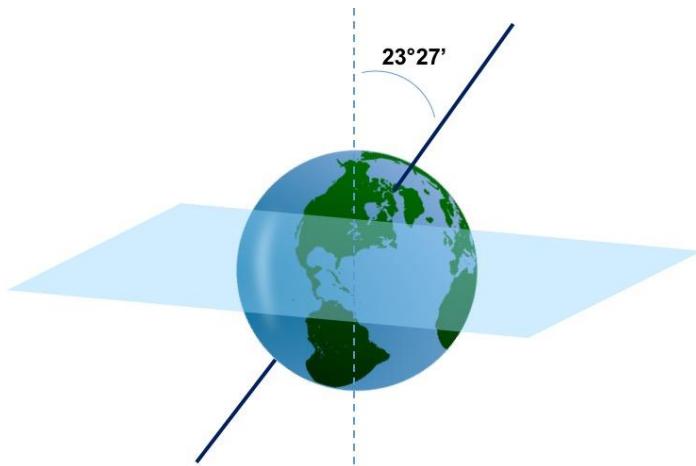


Figure 4. The angle between the Earth's rotation axis and the normal plane of the orbit varies from a minimum of 21° 55' to a maximum of 24° 20', with an average time of approximately 41,000 years.



Figure 5. The Earth's axis performs a double-conic motion, called solar-precession, with a period of about 23,000 years.

In order to perform a quantitative analysis of the registered δO^{18} versus time behavior, which is connected with the Earth temperature values, we have performed both a Fourier analysis of the data during the last 600,000 years, together with and wavelet analysis considering a time window of 5,000,000 years. Figures 6 and 7 report the Fourier and Wavelet diagram of the δO^{18} versus time data [84-95].

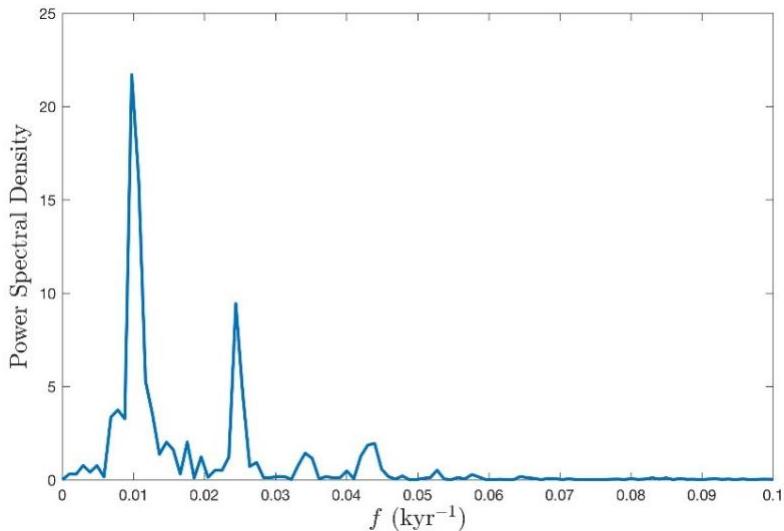


Figure 6. Fourier power spectrum of the δO^{18} versus time behavior during the last 600,000 years.

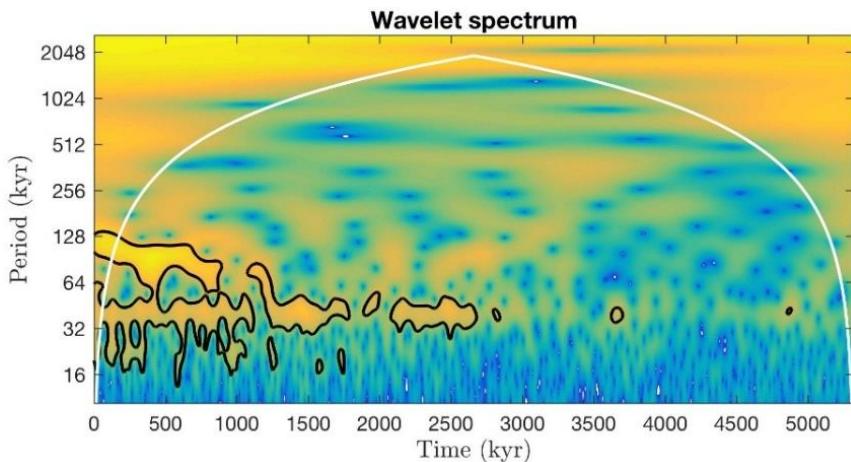


Figure 7. WT power spectrum of the δO^{18} versus time behavior during the last 5,000,000 years.

The Fourier and the wavelet transform analyses confirm the registered temperature periodicities.

What emerges from these analyses is that:

- (i) in the last 500,000 years, it emerges the presence of glacial maxima during which the ice volume was high and the temperatures were low. They repeat with time intervals of around 100,000 years. The 100,000-year time gap separating the glaciations corresponds to that separating two times of extreme eccentricity of the earth's orbit (one of Milankovitch's cycles), when the Earth receives on average a somewhat smaller amount of solar radiation.

- (ii) Between 1.8 and 1.3 million years ago, during 500,000 years, the maximum and the lowest minima repeat more frequently. During this time there are glacial maxima that repeat about every 41,000 years. This time interval is very close to the period in which the cycle of variation of the Earth's axis inclination is performed. This period corresponds to another of Milankovitch's cycles. As in the case of the variation of the eccentricity of the orbit, also the variation of the inclination of the Earth's axis is small -about 3° - but obviously it is enough to trigger a glaciation.

The small variations in the quantity and seasonal distribution of solar radiation during Milankovitch's cycles cannot explain by itself the wide decrease in temperature that marks the transition from an interglacial age to a glacial age. To enhance the effect of these causes there must be a positive feedback or a stochastic resonance effect. This latter term is given to a phenomenon that is marked in nonlinear systems whereby generally a weak signal can be amplified and optimized by the assistance of noise.

This aspect will be dealt in a future work.

CONCLUSION

In this paper we report a case study addressed to graduate students where the results obtained by the application of FT and WT analysis on climate data are presented. Contrarily to FT which furnishes information on the signal periodicities, WT gives details on the time behavior of the signal frequencies content. What emerges from the Fourier and Wavelet analyses is that, in the last 500,000 years, it emerges the presence of glacial maxima with time intervals of around 100,000 years that can be connected with the variation of the eccentricity of the earth's orbit (one of Milankovitch's cycles). Furthermore, between 1.8 and 1.3 million years ago, glacial maxima repeat about every 41,000 years; this time interval corresponds to the cycle of variation of the Earth's axis inclination.

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Chapter 11

A CONCEPTUAL MAP FOR MULTIDISCIPLINARY APPROACHES OF SOFT CONDENSED MATTER PHYSICS IN POSTGRADUATE PROGRAMS

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ABSTRACT

The rapid progress of science and technology in recent years requests a global approach and a synergistic organization of both knowledge and skills for an efficient way of teaching the scientific disciplines. Modern teaching programs request then a synergistic approach which allows to clearly identify the role of each topic within the complex organization of scientific knowledge. In this chapter, we propose a conceptual map for a multidisciplinary approach of the post-graduate programs in soft condensed matter physics, one of the most important field in modern science and technology. Highlighting the synergistic relation and the conceptual interconnection between different parts of the field, may stimulate the exploration of new solutions for a multi- and interdisciplinary integration of knowledge and skills.

Keywords: multidisciplinary teaching approaches, soft condensed matter curriculum, physics conceptual map

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1. INTRODUCTION

The development of specific research approaches based on interdisciplinary studies and innovation investigation represents a crucial element of modern teaching [1]. This holds particularly true in the case of physics education in university post-graduate curricula. The post-graduate programs of physics education, in fact, are involved in developing, implementing, and assessing research-based curricula that are profitably integrated into the various programs of the different scientific disciplines.

Their goals include the improvement of students understanding of physics within the general subjects of the modern nano-technology, through the improvement of student attitudes toward physics applications, as well as the improvement of teacher preparation in the varied and complex world of scientific knowledge. The teaching programs request then a synergistic approach which allows to clearly identify the role of each topic within the complex organization of scientific knowledge [2, 3].

Herein, we propose a conceptual map for the multidisciplinary approaches to soft condensed matter physics (SCMP) in academic postgraduate programs. We highlight the role of the different sub-topics of the soft condensed matter physics, by highlighting the synergistic relation and the conceptual interconnection between different parts of the field. In this respect, the development of a conceptual map may help to efficiently organise the relevant information without the constraints of the single-discipline of traditional curricula. The conceptual map may also stimulate the exploration of new solutions for a multi- and inter-disciplinary integration of knowledge (and skills) which student, at any level, are required nowadays to have.

2. TOWARD AN INTEGRATED APPROACH TO THE INTERDISCIPLINARY CURRICULA IN MODERN SCIENCE

It is well recognised that many of the recent scientific discoveries are made at the interfaces between different fields of science. The principal aim of an interdisciplinary approach to modern teaching is based on an effective integration of the relevant topics of the curriculum, where students can cultivate scientific inquiry through an efficient coordination of both knowledge and skills [2, 3]. The development of the connections between different fields of scientific knowledge is one of the most important ways to shift the paradigms of each different established scientific disciplines.

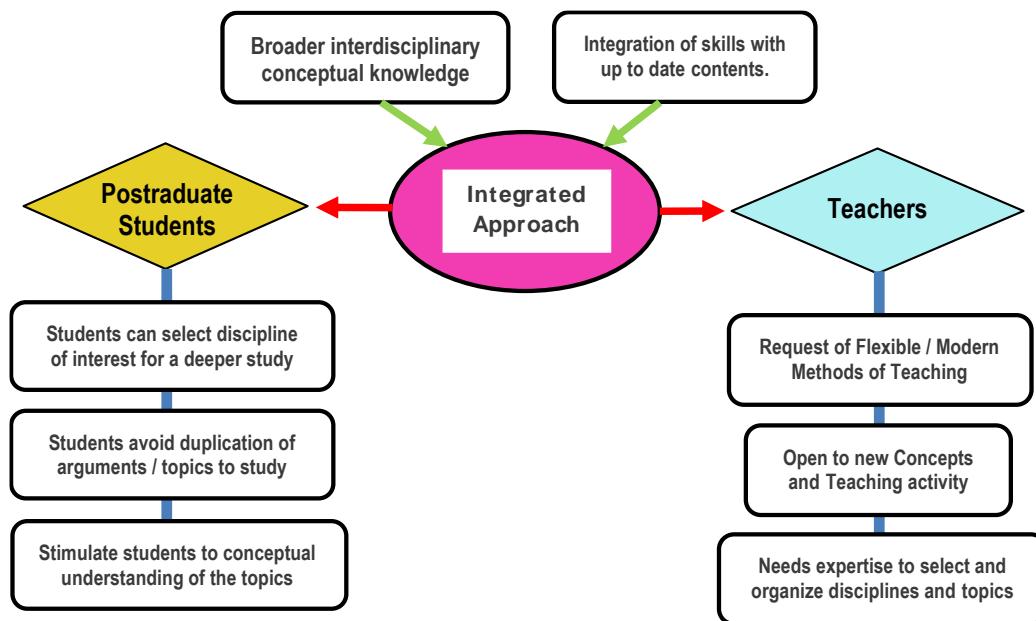


Figure 1. Conceptual Framework for an Interdisciplinary Approach.

Despite the intense debate present in recent years [1-4], the effective integration is still far from having reached its full objective in the different fields of science. An integrated approach to the multi-directional research fields of science, allows learners to study, investigate and organise the relevant information, without the constraints of the single-discipline of the traditional curricula. Moreover the integrated approaches stimulate students to discover the interrelationships between the different curricular topics, while avoiding the duplication of arguments to study (Figure 1). In this sense an integrated approach in SCMP allows the efficient development of skills around a central theme, instead of focusing on learning in isolated curriculum subjects.

From the teachers side, the integrated approach requests modern and flexible methods of teaching and expertise (Figure 1). This needs well equipped and expert teachers who are capable of using modern methods of teaching, especially for what concerns the modern mathematical and computer approaches. A new generation of teachers should be able to systematic effort the challenge to integrate the alternative perspectives of different disciplines into a unified and coherent framework of arguments. Moreover teachers are provided with the special opportunity to work together, by increasing the collegiality, in view of the definition of flexible programs with rigorous cross-disciplinary approaches [1].

3. BASIC CONCEPTS AND EXPERIMENTAL APPROACHES TO THE STUDY OF SOFT CONDENSED MATTER PHYSICS

As previously stated, the integrated approaches allow the efficient development of skills around a central theme, instead of focusing on learning in isolated curriculum subjects. Various strategies can be adopted to efficiently effort the design of highly flexible and modern teaching programs in the fields of modern science and technology. In this section we focus our analysis in one of the most important topics of modern science, i.e., the soft condensed matter physics (SCMP).

The study of condensed matter physics in postgraduate academic programs is mainly motivated by the demand of search for new (nano)materials with unexpected properties. This research field, which is one of the largest subfield of modern physics, seeks to understand the structural and dynamic phenomena arising from the interactions of particles ($\sim 10^{23}$ atoms, molecules or macromolecules) in simple or multicomponent macroscopic materials [5]. This field of physic can be divided in the sub-fields of *hard* and *soft* condensed matter physics.

Hard condensed matter physics (HCMP) deals with materials with higher structural rigidity such as crystalline solids, glasses, insulators, metals, semiconductors and new quantum materials, with the aim to describe their structural, electronic, and transport properties arising from relevant correlations of their basic components at the macro/nano scales of the materials [5].

Soft condensed matter physics (SCMP), on the contrary, describes the macromolecular self-assembly processes and structural organization in the soft-interacting materials [6, 7]. This important field of physics includes the study of colloidal dispersions, soft glasses, liquid crystals, polymers and polyelectrolytes, complex fluids and biological systems (such as bio-membranes and cells). These materials have a vast number of important technological applications in the cross-interdisciplinary fields of material science, biotechnology, nanomedicine, food and personal care products research [6, 7].

The post graduate courses of modern academic programs aim to the development of cross-interdisciplinary skills (tools and methods) to better describe these complex systems. One of the main focus of the research in this field is to discover the relation between the microscopic structural properties of the systems and their bulk mechanical or collective behaviour. As reported in Figure 1, the main experimental methods for the investigation of the structural properties of (multicomponent) systems in SCMP are the *spectroscopic (and scattering) techniques* and the *image (microscopy) techniques*. Those techniques represent the most employed experimental approaches for a large variety of soft-materials in the interdisciplinary fields of biotechnology, nanomedicine and in material and environmental science [7-9].

Both the two main approaches use a radiation source as the interaction probe and a detection system that collect the response of the material system [7, 8] resulting from the probe action. While the microscopy techniques furnish high spatial resolution structural pictures in real space [10], spectroscopy and scattering methods provides important statistical (ensemble-averaged) information of material systems in the reciprocal space. The relevant wave-vectors \mathbf{k} probed correspond to length scales ranging from few nanometers to fractions of millimetre [8, 11-15]. On a more general background, the study of the interaction of the electromagnetic radiation with the material systems is described by a generalised *dynamic structure factor* $S(\mathbf{k}, \omega)$ that describes the molecular motion (i.e., rotations, vibrations, translations) of nanostructured molecular systems of the SCMP in terms of the scattering wavevector \mathbf{k} , and the frequency ω of the detected radiation response [8, 9].

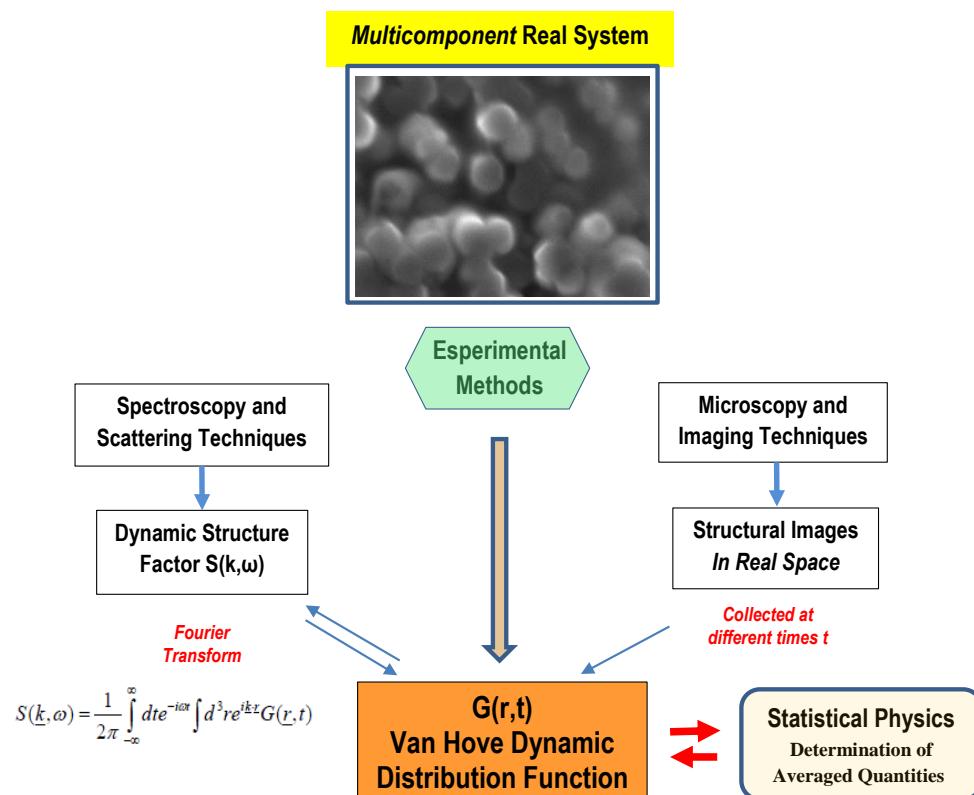


Figure 2. Main experimental approaches to the study of soft condensed matter physics.

For example, the dynamic structure factor $S(\mathbf{k}, \omega)$ is probed by the inelastic neutron scattering experiments, through the measurement of the scattering differential cross section $(d^2\sigma/d\Omega d\omega) = a^2(E_f/E_i)^{1/2} \cdot S(\mathbf{k}, \omega)$, (where E_f and E_i are the initial and final neutron energies) [8]. As reported in the conceptual map of Figure 2, the *van Hove*

distribution function $G(r, t)$ plays a central role in the description of the main features of spectroscopic (and scattering) techniques.

This function represents a (real-space) dynamical correlation function that characterizes the space-time distributions of pairs of particles of a multicomponent system (such as a fluid or a general material system) [16]. It describes the probability of finding a particle at position r at time t , given that a different (or the same) particle was located at the origin ($r = 0$) at the initial time ($t = 0$) [16].

Apart the spectroscopic (and scattering) approaches, in recent years the advent of modern microscopy techniques allow to characterize with high spatial resolution the structure of many multicomponent systems of SCMP in real space [10]. As evidenced in Figure 2, a conceptual link to those apparently unrelated techniques can be found in the definition and computation of the van Hove distribution function $G(r, t)$.

The function $G(r, t)$, that summarises the structural properties of the material system (spatial correlation of their main components), can be computed starting by the analysis of images collected in the real space (at different times). An interesting example of the computation of the function $G(r, t)$ is given by the *digital fourier microscopy* (DFM) approach for the study of the dynamics of soft materials [17].

In this respect, the main weak non-covalent forces (such as hydrogen bonding, electrostatic interactions, van der Waals forces, steric interactions) acting on constituents particles of SCMP systems, play an important role in determining the structural and dynamic properties of soft materials [18-22].

4. THEORETICAL APPROACHES FOR THE STUDY OF SCMP

Molecular dynamic (MD) simulations and analytical theories represent the main theoretical approaches for the study of multidisciplinary curriculum in SCMP.

Molecular dynamics (MD) simulations methods are able to describe a wide range of soft matter processes, addressing a variety of interdisciplinary issues including conformations of polymers and proteins, relevant bio-conjugates and material complexes [23, 24]. The MD approach is particularly important for the study of self-assembly processes of nanoparticles and their interaction with biological systems, like carbohydrates, proteins, lipid membrane and cells [23-25]. As evidenced in Figure 3, the form of the inter-particles interaction plays a prominent role in determining, with its mathematical expression, the numerical solution of the molecular dynamics approach. For this reason different molecular dynamic (MD) frameworks and solution schemes has been implemented in a wide range of investigations, including full atoms or coarse grained MD, Monte Carlo or Ab initio molecular dynamic [23-25].

On the other side, the use of analytical theories furnishes a powerful tool for a mathematical representation of complex phenomena in SCMP, by the calculation their

potential observable properties (Figure 3). Together with basic thermodynamic and statistical theories, different theoretical approaches have been developed for a wide range of investigations in the different research fields connected with SCMP, including mean field theory (MFT), density functional theory (DFT) and integral equations theories (IET) just to name a few [26-32].

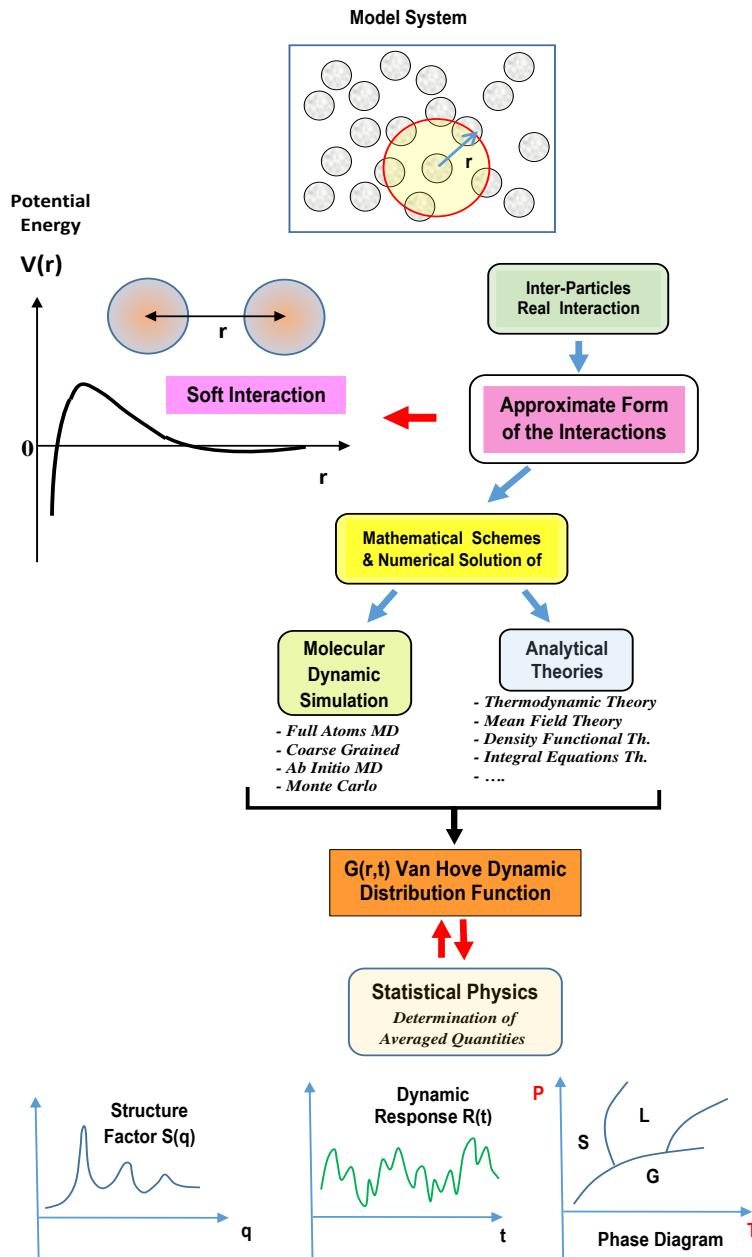


Figure 3. A conceptual map describing the main theoretical methods for the study of the properties of soft interacting materials.

As in the case of molecular dynamic simulation, the analytical theories often request a simple mathematical form for the solution of the main relevant interactions involved. The employment of suitable numerical solution schemes allows the exploration of approximate solution of the investigated many-particle, complex systems of SCMP.

For example in integral equations approaches the solution of the O-Z integral equation is possible only after appropriate solution schemes (so called closure relations), such as the hypernetted chain (HNC), mean spherical approximation (MSA), Percus-Yevick (P-Y) [33-35]. The integral equations theoretical approach has been employed to investigate the strength and range of interparticle interactions in different material systems of SCMS including amphiphiles micelles, dendrimers, lipid vesicles and proteins [36-40].

5. COMBINED THEORETICAL AND EXPERIMENTAL APPROACHES IN THE STUDY OF SCMP

As future research in nanotechnology and material science will move toward the investigation of increasingly complex, hierarchical systems [41-46], the use of combined approaches, that associate a deep theoretical analysis in connection to the experimental investigations, will become imperative. Combined theoretical-experimental approaches has been recently applied in an increasing number of soft materials investigations with the aim to elucidate the design rules for the complex self-assembled nanostructured systems of SCMP [47-53]. For example molecular dynamics simulation techniques have been widely employed in connection with experimental methods such as X-ray crystallography [52], NMR [53], infrared spectroscopy (IR) [54], and small angle (X-rays and Neutron) scattering [55-57] investigations. Within this approach the molecular interactions can be directly inferred from the best simulated molecular system [55-56].

Similarly, also the analytical theories are involved in the combined theoretical-experimental investigations of material systems of SCMP. Theoretical approaches greatly help the structural interpretation of the experimental results as well as the identification of the key properties that primarily influence the structural and dynamic properties of SCMP materials. In this respect, the direct comparison of the crucial parameters obtained from theoretical and experimental approaches request the employment of suitable mathematical models and novel computational efforts [58-62].

The ability to design new experiments and to draw hypotheses within a research investigation represents a crucial step for the scientific work of the new generation of postgraduate students and young researchers. This requests a broader interdisciplinary conceptual knowledge in connection with an integration of skills with up to date contents.

6. LINK BETWEEN THEORY AND EXPERIMENTS: THE CENTRAL ROLE OF THE STATISTICAL PHYSICS

For an effective and efficient teaching of the SCMP topics, the planning of the integrated units is essential. In this respect a specific issue must be dedicated to a rigorous treatment of the statistical physics methods. Statistical physics plays a central role in academic curriculum of SCMP as it allows the description of the collective behaviours of large ensembles of interacting objects. Moreover, statistical distribution functions (such as the van Hove function) represent the fundamental link between theory and experiments. Measurable parameters and properties obtained by experimental approaches can be obtained as averaged quantities of the relevant distribution functions (see Figure 3) and can be calculated within the framework of the different theoretical approaches. The employment of statistical physics approaches facilitated a growing understanding of fundamental processes such as the main self-assembly mechanisms underlying many advanced materials in nanoscience [63-68]. This allows to identify the number of physics concepts of interest within the multi- and inter-disciplinary contests, thus providing the proper tools and skills to investigate progressively complex nano- and super-structures in the rapidly expanding field of material science and nanotechnology [69-74].

Within this contest, the planning of the teaching units of the different topics of SCMP requests then a suitable link to well defined topics of statistical physics. This link provides an adequate theoretical explanation of the structural properties and their connected spatial/temporal processes involved in large variety of systems, in the cross-interdisciplinary fields of biology, nanomedicine and material science. The interdisciplinary character of these topics will stimulate students to reflect on the cross-disciplinary thinking and the need for a fruitful collaboration between expertise coming from the experimental and theoretical world [75-77].

CONCLUSION

The rapid progress of science and technology experienced in the last decades has changed the objectives and the way of teaching scientific disciplines. Modern global approaches within science university curricula request, in fact, a synergistic organization of both knowledge and skills for an efficient integration of the relevant information of the different involved topics.

In this perspective, we propose a conceptual map for the multidisciplinary approaches of soft condensed matter physics in academic postgraduate programs. We point out the role of the main approaches of the soft condensed matter physics by

highlighting their relation and their conceptual interconnections. A central role is given by the statistical physics, as the study of the statistical distribution functions allows a useful connection between theory and experiments.

Within this context teachers need adequate preparation in both content and instructional strategies in order to face the challenges for a multi- and inter-disciplinary integration of knowledge in science. A new generation of teachers that are able to systematic effort the integration of the different disciplines into a unified and coherent framework of arguments.

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Chapter 12

GENERALIZED WIEN'S DISPLACEMENT LAW OF THERMAL RADIATION OF A REAL-BODY

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ABSTRACT

The expression for “generalized” Wien’s displacement law of thermal radiation of a real-body is represented using a limited number of frequency moments. In the case of blackbody radiation, this expression is transformed into the well-known the Wien displacement law. The temperature dependence of the “generalized” Wien displacement law for the several metals, carbides, luminous-flames, and the quasi-periodic microstructured silicon coated with 100 nm thick Au film has been studied. In the case of high temperatures, it is shown that Wien’s displacement law decreases linearly with increasing the temperature. This means that the metals and carbides studied belong to the same universality class. The emitted thermal radiation of the luminous flames, when $K_V L \ll 1$, belongs to the universality class as thermal radiation of a blackbody.

At low temperatures, the temperature dependence of the “generalized” Wien displacement law for the quasiperiodic microstructured silicon coated with 100 nm thick Au film is more complex. The true temperatures of the materials under study can be determined by measuring the position of the maximum of the spectral energy density. The uncertainty in determining the true temperature in these cases is less than 2%.

Keywords: generalized Wien’s displacement law, true temperature, metals, carbides, luminous flames, microstructured silicon coating with Au film

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1. INTRODUCTION

When a lecturer conducts a course of thermodynamics or statistical physics on a topic related to the thermal radiation of a blackbody, students very often ask how we can generalize the well-known Wien displacement law to the case of thermal radiation of a real-body? Or, in other words, can we determine the true temperature of real-body radiation by measuring the maximum of the spectral energy density?

This chapter is devoted to obtaining answers to these questions.

It is well known that the direct method of determining the temperature of blackbody radiation is the Wien displacement law. By measuring the position of the maximum of the spectral density of blackbody radiation, it is possible to determine the temperature of the emitted object. By using this law, the temperature of the Cosmic Microwave Background (CMB) radiation [1], solar and other cosmic objects was defined.

Unlike blackbody radiation, to determine the true temperature of a real body, it is necessary to know the frequency dependence of the spectral emissivity $\varepsilon(\nu, T)$. Therefore, a great number of experimental studies were focused on the measurement of the spectral emissivity for various materials [2, 3].

Multiwavelength emissivity models were also proposed in [4, 5]. The true temperature of a real-body can be measured using optical multispectral radiation thermometers in conjunction with multiwavelength emissivity models. There are other emissivity models that base on fundamental physical principals. Such models are Maxwell, Hagen-Ruben and Edwards [6, 7].

A non-contact method determining the true temperature of a real-body from “generalized” Wien’s displacement law was proposed in [8]. The method was proven on the spectra of the thermal radiation of tungsten, tantalum, molybdenum, luminous flames, ZrB₂-SiC-based ultra-high temperature ceramics and zirconium, hafnium, and titanium carbides [8-15]. The accuracy in the determination of the steady-state temperature in these cases does not exceed 2%.

This chapter provides a detailed review of the research related to this topic.

2. FUNDAMENTAL RELATIONS

The method of moments for constructing a “generalized” Wien displacement law for thermal radiation of a real-body was proposed in [8]. The position of the maximum of the radiant spectral energy density of a real-body can be presented in the form:

$$\nu_{max} = \beta(1 - \gamma), \quad (1)$$

where

$$\beta = \frac{S_1}{S_0}, \quad \gamma = \frac{S_0 \bar{S}_3}{2S_1 \bar{S}_2}. \quad (2)$$

Here:

$$S_n(T) = \int_{\nu_1}^{\nu_2} \nu^n I(\nu, T) d\nu, \quad (3)$$

$$\bar{S}_n(T) = \int_{\nu_1}^{\nu_2} (\nu - \bar{\nu})^n I(\nu, T) d\nu, \quad (4)$$

are the initial Eq. (3) and central Eq. (4) moments of the distribution function $I(\nu, T)$, $n = 0, 1, 2, 3, \dots, k$ is the order of the moments; $\bar{\nu} = \frac{S_1}{S_0}$.

$$\bar{S}_0 = S_0, \quad (5)$$

$$\bar{S}_1 = 0, \quad (6)$$

$$\bar{S}_2 = S_2 - \frac{S_1^2}{S_0}, \quad (7)$$

$$\bar{S}_3 = S_3 - 3 \frac{S_1 S_2}{S_0} + 2 \frac{S_1^3}{S_0^2} \quad (8)$$

The radiant spectral energy density of a real-body having emitting continuous spectra can be represented in the form,

$$I(\nu, T) = \varepsilon(\nu, T) I^P(\nu, T), \quad (9)$$

where $\varepsilon(\nu, T) = \frac{I(\nu, T)}{I^P(\nu, T)}$ is the spectral emissivity of a real-body and $I^P(\nu, T)$ at temperature T is given by the Planck law [16]:

$$I^P(\nu, T) = \frac{8\pi h}{c^3} \frac{\nu^3}{e^{\frac{h\nu}{k_B T}} - 1}, \quad (10)$$

where k_B is the Boltzmann constant and h is the Planck constant.

According to Eq. (1), the “generalized” Wien displacement law has the following form:

$$X_{max} = \frac{hv_{max}}{k_B T} = \frac{h}{k_B T} \beta(1 - \gamma) \quad (11)$$

According to Eq. (11), the true temperature of thermal radiation of a real-body is determined by the following expression:

$$T = \frac{h}{X_{max} k_B} \beta(1 - \gamma) \quad (12)$$

Let us note the following. The expressions Eq. (3) and Eq. (4) can be transformed to the wavenumber ($\tilde{\nu} = \frac{v}{c}$) or wavelength ($\lambda = \frac{c}{v}$) domains. For example, for 0th moments, we should use the following relationships:

$$\int_{\nu_1}^{\nu_2} \varepsilon(\nu, T) I^P(\nu, T) d\nu = - \int_{\lambda_1}^{\lambda_2} \varepsilon(\lambda, T) I^P(\lambda, T) d\lambda = \int_{\tilde{\nu}_1}^{\tilde{\nu}_2} \varepsilon(\tilde{\nu}, T) I^P(\tilde{\nu}, T) d\tilde{\nu} = I(x_1, x_2, T) \quad (13)$$

The calculated values of the integrals in Eq. (13) in various ranges from x_1 to x_2 for different domains when $\varepsilon(\nu, T)$ are presented in [17].

The arbitrary variable x is represented in all three domains as follows:

$$x = \frac{hv}{k_B T} = \frac{hc}{\lambda k_B T} = \frac{h\tilde{\nu}}{k_B T} \quad (14)$$

The spectral energy density of blackbody radiation in different domains is presented as:

Wavelength domain λ :

$$I^P(\lambda, T) d\lambda = - \frac{8\pi hc}{\lambda^5 \left[\exp\left(\frac{hc}{\lambda k_B T}\right) - 1 \right]} \quad (15)$$

Wave number domain $\tilde{\nu}$:

$$I^P(\tilde{\nu}, T) d\tilde{\nu} = \frac{8\pi hc \tilde{\nu}^3}{\left[\exp\left(\frac{h\tilde{\nu}}{k_B T}\right) - 1 \right]} d\tilde{\nu} \quad (16)$$

As seen, the results of integrals in Eq. (13) are identical because any variable substitution does not affect the value of the calculated integrals. Thus, the solution is independent on the choice of the domain because it represents the same physical quantity. As for other moments, more research should be done.

Let us consider the thermal radiation of a blackbody. In this case $\varepsilon(\nu, T) = 1$. The initial Eq. (3) and central Eq. (4) moments of the Planck function in the finite spectral range can be presented using the polylogarithmic representation,

$$S_n(x_1, x_2) = \int_{\nu_1}^{\nu_2} \nu^n I^P(\nu, T) d\nu = \frac{8\pi(k_B T)^{4+n}}{c^3 h^{3+n}} (3+n)! A_n(x_1, x_2), \quad (17)$$

where

$$\tilde{A}_n(x_1, x_2) = [P_{3+n}(x_1) - P_{3+n}(x_2)]. \quad (18)$$

Here $P_{3+n}(x)$ is defined as

$$P_{3+n}(x) = \sum_{s=0}^{3+n} \frac{(x)^s}{s!} \text{Li}_{4+n-s}(e^{-x}) \quad (19)$$

where

$$\text{Li}_{4+n-s}(e^{-x}) = \sum_{k=1}^{\infty} \frac{e^{-kx}}{k^{4+n-s}}, |e^{-kx}| \quad (20)$$

is the polylogarithm functions [18].

Using Eqs. (11, 17), the polylogarithmic representation of the Wien displacement law takes the following form:

$$X_{max} = \frac{4(P_4(x_1) - P_4(x_2))}{P_3(x_1) - P_3(x_2)} [1 - \gamma(S_0(x_1, x_2), S_1(x_1, x_2), \bar{S}_2(x_1, x_2), \bar{S}_3(x_1, x_2))] \quad (21)$$

According to Eq. (21), the temperature of thermal radiation of a blackbody in a finite range of frequencies is determined by the formula

$$T = \frac{h\nu_{max}(P_3(x_1) - P_3(x_2))}{4(P_4(x_1) - P_4(x_2))} [1 - F(S_0, S_1, \bar{S}_2, \bar{S}_3)]^{-1} \quad (22)$$

As can be seen from Eq. (22), to determine of the temperature, the value of ν_{max} should be measured experimentally.

3. BLACK BODY RADIATION

It is well-known [16] that the Wien displacement law of blackbody radiation can be obtained by solving the transcendental equation $\left(\frac{\partial I^P(\nu, T)}{\partial \nu} = 0, \frac{\partial^2 I^P(\nu, T)}{\partial \nu^2} < 0 \right)$ numerically. As a result, the Wien displacement law of blackbody radiation has the following value:

$$X_{max}=2.8214 \quad (23)$$

Now let us show that the generalized Wien displacement law of blackbody radiation, Eq. (21) represented by combination of frequency moments has the same value as Eq. (23). To calculate the integrals for determining the initial and central moments Eqs. (3, 4, 17), we should use the semi-infinite interval $v_1 = 0$, and $v_1 = \infty$. In this case, since $P_{3+n}(\infty) = 0$ and $P_{3+n}(0) = \text{Li}_{4+n}(1)$, $S_n(0, \infty)$ takes the form

$$S_n(0, \infty) = \frac{8\pi(k_B T)^{n+4}}{c^3 h^{3+n}} (3+n)! \text{Li}_{4+n}(1) \quad (24)$$

Here $\text{Li}_{4+n}(1) = \zeta(n+5)$, $\zeta(n+5)$ is the Riemann zeta function.

Using Eq. (24), the Eq. (21) can be written as

$$X_{max} = \beta' [1 - \gamma'(S_0(0, \infty), S_1(0, \infty), \bar{S}_2(0, \infty), \bar{S}_3(0, \infty))] \quad (25)$$

Here

$$\beta' = \frac{4(P_4(0) - P_4(\infty))}{P_3(0) - P_3(\infty)} = \frac{4\text{Li}_5(1)}{\text{Li}_4(1)} = 3.83231 \quad (26)$$

and

$$\gamma' = 0.26103 \quad (27)$$

Substituting the values of β' and γ' in Eq. (21), we finally obtain

$$X_{max} = 2.8319 \quad (28)$$

As we see, Eq. (28) negligibly differs from the well-known Wien displacement law ($X_{max}=2.8214$). The uncertainty in this case does not exceed 1%.

In conclusion, we note that an analogous result for the Wien displacement law was obtained in [10-12], using the following integral:

$$\int_0^\infty \frac{x^n}{e^x - 1} dx = \Gamma(n+1)\zeta(n+1), \quad (29)$$

Here $\Gamma(n+1)$ is gamma function and $\zeta(n+1)$ is the Riemann function (both these functions have been tabulated).

4. REAL-BODY THERMAL RADIATION

Below we will consider several examples illustrating that the true temperature of the thermal radiation of a real-body can be obtained from experimental data using Eq. 12.

4.1. Soot-Forming Flames

According to [19, 20], the monochromatic emissivity $\varepsilon(\nu, T)$ of luminous flames, when $K_\nu L \ll 1$, is given by the following formula:

$$\varepsilon(\nu, T) = \varepsilon_0 \nu^\alpha, \quad (30)$$

here K_ν is the absorption coefficient for the frequency ν , L is thickness of the absorbing layer, and α takes different values for different flames (see Table 1).

The n^{th} frequency moment for the radiant spectral density with the help of Eq. (3), Eq. (4) and Eq. (30) takes the form:

$$S_n = A_n T^{n+\alpha+4}, \quad A_n = \frac{8\pi\varepsilon_0}{c^3} \frac{k^{4+n+\alpha}}{h^{3+n+\alpha}} \int_0^\infty \frac{x^{3+n+\alpha}}{e^x - 1} dx \quad (31)$$

By combining the results from Eq. (31) and Eq. (1), the expression for the true temperature of luminous flames can be obtained in the form:

$$T = A' \frac{h\nu_{\max}}{k} \quad (32)$$

The coefficient A' is defined by the expression:

$$A' = \frac{A_1}{A_0} \left(1 + \frac{A_0 A_3}{2 A_1 A_2} \beta \right), \quad (33)$$

where

$$\beta = \frac{\left[1 - \frac{3A_1 A_2}{A_0 A_3} \left(1 - \frac{A_1^2}{A_0 A_2} \left(1 - \frac{1}{3A_0} \right) \right) \right]}{1 - \frac{A_1^2}{A_0 A_2}} \quad (34)$$

The value of coefficients A' for different flames is given in Table 1.

Table 1. Calculated values of the constant A' .Values of α are taken from [20]

FLAME	α	$A', 10^{-1}$
Acetone	1.43	2.29
Amyl acetate	1.39	2.31
Caol-gas/air	1.29	2.41
Benzene/air	1.23	2.43
Nitrocellulose	1.14	2.51
Benzene/NO	1.05	2.55
Acetylene/air	0.66 to 0.75	2.69 to 2.64

As can be seen from Eq. (32), when determining the luminous flame temperature from experimental data, only accurate measurements of the maximum of the spectral radiation are needed.

Let us consider in more detail an example of an acetone flame ($\alpha = 1.43$). According to Eq. (31), the coefficients A_n in the Eq. (33) and Eq. (34) are equal to:

$$A_0 = 19.08 \cdot \frac{B(k)^{5.43}}{h^{4.43}}, \quad A_1 = 105.27 \cdot \frac{B(k)^{6.43}}{h^{5.43}}$$

$$A_2 = 668.23 \cdot \frac{B(k)^{7.43}}{h^{6.43}} \text{ and } A_3 = 4919.53 \cdot \frac{B(k)^{8.43}}{h^{7.43}} \quad (35)$$

$$\text{Here } B = \frac{8\pi\varepsilon_0\Gamma(0.43)}{c^3}.$$

Combining Eqs. (32 and 35), the temperature of thermal radiation of amyl acetate is

$$T = A' \frac{hv_{max}}{k} \quad (36)$$

where the coefficient $A' = 2.29 \cdot 10^{-1}$. As seen from Eq. (36), for determining the true temperature of thermal radiation of amyl acetate, the position of the maximum of the spectral energy density should be measured experimentally.

In conclusion, we note that a similar law of dependence between T and v_{max} is obtained for luminous flames and a black body. This means that the emitted radiation of luminous flames in the case when $K_vL \ll 1$ and black body radiation belong to the same universality class.

4.2. Metals at High Temperatures

Now let us consider the temperature dependence of the “generalized” Wien displacement law Eq. (11) for metals.

Unlike to luminous-flames, the emissivity $\varepsilon(\nu, T)$ for molybdenum at different temperatures is given by Tables. In [2] the experimental values of the spectral emissivity $\varepsilon(\nu, T)$ for molybdenum at different temperatures are presented. Using the Simpson rule [21], the values of the S_0 , S_1 , S_2 , and S_3 moments of the spectral energy density at different temperatures are calculated and presented in Table 2. The temperature dependence of the “generalized” Wien displacement law for molybdenum is studied and represented in Figure 1. As can be seen in Fig. 1, the “generalized” Wien displacement law X_{max} is approximated with a good accuracy by the equation

Table 2. Temperature dependence of the initial moments $S_n = \int_{\nu_1}^{\nu_2} \nu^n I(\nu, T) d\nu$ of the radiant spectral energy density for molybdenum

T (K)	$S_0 \times 10^{-4}$ (J·m ⁻³)	$S_1 \times 10^{11}$ (J·m ⁻³ ·s)	$S_2 \times 10^{25}$ (J·m ⁻³ ·s ⁻²)	$S_3 \times 10^{39}$ (J·m ⁻³ ·s ⁻³)
1200	1.201	0.169	0.278	0.531
1400	3.176	0.504	0.943	2.057
1600	6.936	1.221	2.561	6.295
1800	13.450	2.599	6.032	16.485
2000	23.910	5.022	12.750	38.240

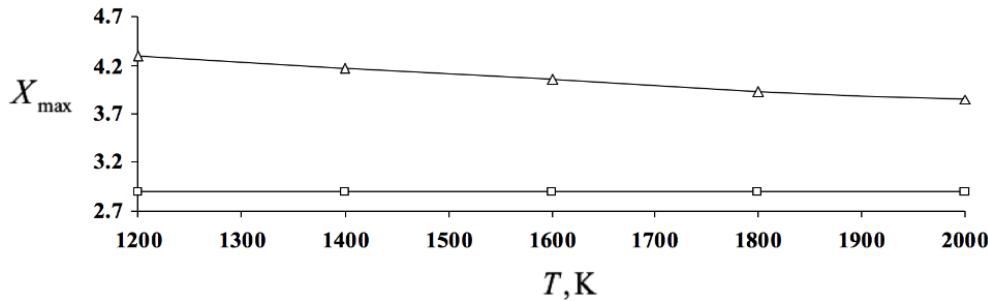


Figure 1. Investigation of the “generalized” Wien displacement law for molybdenum: □ - black body; Δ - molybdenum.

$$X_{max} = \frac{h\nu_{max}}{kT} = a' - b'T \quad (37)$$

where $a' = 4.99$ and $b' = 5.75 \times 10^{-4} K^{-1}$. The constants a' and b' are estimated using the least-squares method. From Eq. (37), the true temperature of thermal radiation of molybdenum has the following expression:

$$T = c' \left[1 - (1 - d'\nu_{max})^{\frac{1}{2}} \right] \quad (38)$$

where $c' = 8.67 \times 10^3 K$ and $d' = 4.44 \times 10^{-15} s$.

As can clearly be seen from Eq. (38), for determining the true temperature of thermal radiation of molybdenum, the position of the maximum of the radiant spectral density should be measured experimentally.

Now let us compare the calculated value for the true temperature of molybdenum Eq. (38) with the experimental data. In accordance with the experimental data [2], at the temperature $T = 2000K$, the value of $v_{max} \approx 0.93 \times 10^{14}s^{-1}$. After substituting the experimental value v_{max} in Eq. (38), the calculated value of the temperature for molybdenum is equal to $T = 2027K$. As seen, the uncertainty in the determination of the true temperature in this case is no larger than 2%.

4.3. Carbides at High Temperatures

Now let us investigate the temperature dependence of the generalized Wien displacement law for stoichiometric carbides.

In [22], the experimental values of the normal spectral emissivity $\varepsilon(v, T)$ for stoichiometric zirconium carbide at high temperatures for wavelengths between $0.65\mu\text{m}$ and $6.0\mu\text{m}$ are presented. Using the Simpson rule [21], the calculated values of β and γ in Eq. (1) at different temperatures are presented in Table 3.

According to Table 3, the “generalized” Wien displacement law has been investigated at different temperatures and is shown in Figure 2.

As seen in Fig. 2, X_{max} for the stoichiometric zirconium carbide decreases linearly with increasing temperature and is approximated with a high degree of accuracy by a linear equation,

$$X_{max} = \frac{hv_{max}}{kT} = a' - b'T, \quad (39)$$

Table 3. Temperature dependences of the constants β and γ , and the initial 0th moments $S_0 = \int_{v_1}^{v_2} I(v, T)dv$ of the spectral energy density for zirconium carbide

Material	Zirconium Carbide	β	γ
T, K	$S_0 \times 10^3 (J \cdot m^{-3})$		
2300	8.068	4.378	0.123
2400	9.987	4.306	0.115
2500	12.157	4.234	0.108
2600	14.624	4.164	0.101
2700	17.398	4.096	0.094
2800	20.505	4.030	0.087
2900	23.909	3.966	0.080

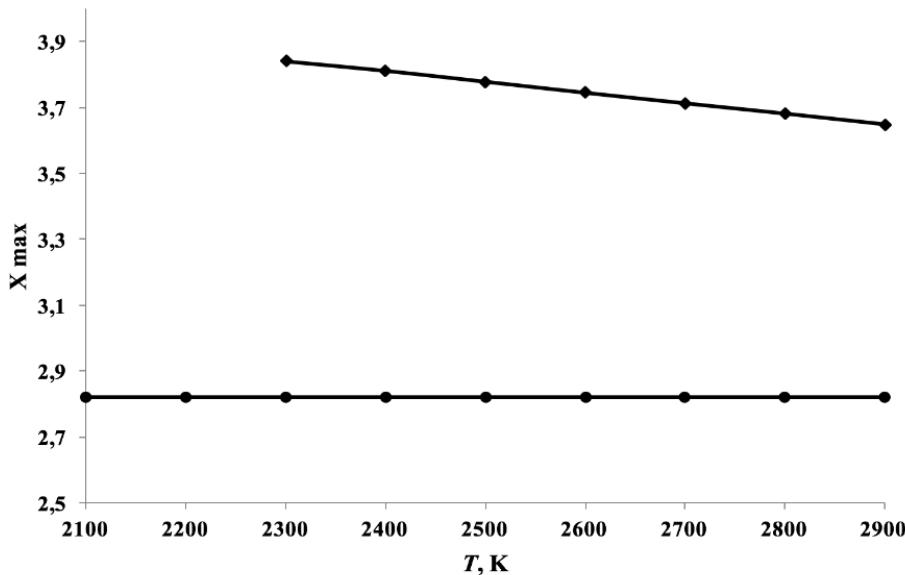


Figure 2. Investigation of the “generalized” Wien displacement law for stoichiometric zirconium carbide: ♦ - zirconium carbide; ● - black body.

Where $a' = 4.83$ and $b' = 4.01 \times 10^{-4} K^{-1}$. The constants a' and b' are estimated using the least-squares method. From Eq. (39), the true temperature of thermal radiation of the stoichiometric zirconium carbide is obtained in the following form:

$$T = c' \left[1 - (1 - d' v_{max})^{\frac{1}{2}} \right] \quad (40)$$

where $c' = 6.03 \times 10^3 K$ and $d' = 3.293 \times 10^{-15} s^{-1}$.

As seen from Eq. (40), to determine the true temperature of thermal radiation of the stoichiometric zirconium carbide, the experimental value of the position of the maximum of the spectral energy density is necessary.

In the case of the stoichiometric zirconium carbide, the experimental value of the position of the maximum of the spectral energy density at the temperature $T = 2900 K$ is as follows: $v_{max} = 2.2199 \cdot 10^{14} s^{-1}$. Substituting this value into Eq. (40), the calculated true temperature is $T = 2902.6 K$. As can be seen, the calculated true temperature is in good agreement with the experimental data.

In conclusion, it is important to note that a similar law of the relationship between the true temperature T and the position of the maximum v_{max} of the spectral energy density was obtained for tantalum, tungsten, molybdenum, stoichiometric zirconium, titanium and hafnium carbides [9, 11, 12, 13]. This means that the emitted radiations of molybdenum, tantalum, tungsten, and stoichiometric zirconium, titanium and hafnium carbides belong to the same universality class.

The constants c' and d' in Eq. (40) for stoichiometric hafnium, titanium, and zirconium carbides differ for each other and the same constants in [9, 11, 12, 13]. It appears that this difference is related to the difference in the compositions, surface states and its degrees of oxidation. This question will be the focus of our future research.

4.4. Microstructured Silicon Coated with Au Film

Now let us investigate the temperature dependence of the “generalized” Wien displacement law for microstructured silicon coated with Au film. In [23], the experimental values of the normal spectral emissivity $\varepsilon(v, T)$ for the microstructured silicon coated with Au film at different temperatures in the wavelengths range between $3.277\mu\text{m}$ and $24.926\mu\text{m}$ are presented. Using these data and Monte Carlo method [21], the temperature dependences of the constants β and γ are calculated and presented in Table 4.

The generalized Wien displacement law at different temperatures has been investigated. The results are represented in Figure 3.

As can be seen in Fig. 3, X_{max} decreases when the temperature increases and is approximated with a high degree of accuracy by the cubic equation,

$$X_{max} = \frac{hv_{max}}{k_B T} = a' + b'T + c'T^2 + d'T^3, \quad (41)$$

Table 4. Temperature dependences of the constants β and γ , and the initial 0th moments $S_0 = \int_{v_1}^{v_2} I(v, T) dv$ of the spectral energy density for microstructured silicon coated with Au film

Materials	Microstructured silicon coated with Au film	β	γ
$T(K)$	$S_0(10^{-5} \cdot J \cdot m^{-3})$	β	γ
373	1.301682	5.819556	0.083239
423	2.708670	5.598718	0.048947
473	4.990872	5.360554	0.020984
523	8.561161	5.127452	-0.002299
573	13.646327	4.891151	-0.020877
623	20.516267	4.657504	-0.034726
673	29.040024	4.430447	-0.045040

Where $a' = 2.867455$, $b' = 1.466553 \times 10^{-2} K^{-1}$, $c' = -2.613842 \times 10^{-5} K^{-2}$ and $d' = 1224249 \times 10^{-8} K^{-3}$. The constants a', b', c' and d' are estimated using the least-squares method. For instance, the calculated values of the “generalized”

Wien displacement law Eq. (11) are as follows: (a) $T = 373K$, $X_{max} = 5.3351$; (b) $T = 573K$, $X_{max} = 4.9932$; (c) $T = 673K$, $X_{max} = 4.6299$.

According to Eq. (41), the true temperature can be obtained by solving the following fourth - degree equation [21]:

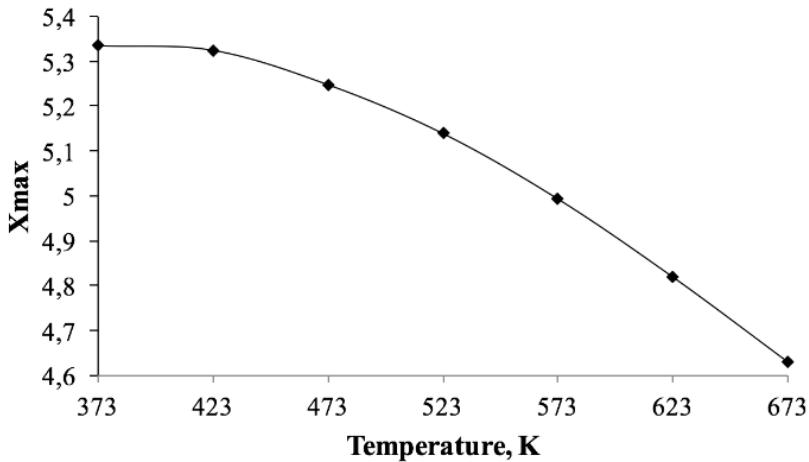


Figure 3. Investigation of the “generalized” Wien displacement law for the microstructured silicon coated with Au film.

Table 5. Comparison analysis in determining the true temperatures of the thermal radiation of microstructured silicon coated with Au film from the “generalized” Wien displacement law

Experimental Values $T(K)$	Calculated values using Eq. 42 $T(K)$
373.00	370.91
423.00	420.34
473.00	471.59
523.00	519.99
573.00	570.23
623.00	619.99
673.00	670.91

$$T^4 + \frac{c'}{d'} T^3 + \frac{b'}{d'} T^2 + \frac{a'}{d'} T - \frac{h v_{max}}{k_B d'} = 0 \quad (42)$$

In Table 5, the calculated values of the true temperatures obtained from Eq. (42) and experimental values are presented.

As seen, the calculated true temperatures are in good agreement with experimental data.

As can clearly be seen from Eq. (42), the experimental value of the position of the maximum of the spectral energy density is required to determine the true temperature of microstructured silicon coated with Au Film.

CONCLUSION

In this chapter we propose the solution of the following questions:

- a) How can we generalize the well-known Wien displacement law in the case of thermal radiation of a real body?

or

- b) Is it possible to determine the true temperature of thermal radiation of a real-body by measuring the maximum of the spectral energy density?

The answer to these questions is as follows. The position of the maximum of the radiant spectral energy density is represented through a combination of a limited number of initial and central moments. The initial and central moments are the integral characteristics of the system. The true temperature is determined from the temperature dependence of generalized Wien's displacement law. The latter in the case of blackbody radiation turns into a well-known expression for the Wien displacement law. The uncertainty of this method is greater when the spectral emissivity is properly measured with good accuracy. The uncertainty is even greater when the initial and central moments are calculated with a high degree of accuracy. For determining the true temperature of thermal radiation of real-bodies, the experimental values of the position of the maximum of the spectral energy density are necessary.

Applicability of this method was demonstrated on thermal radiation of: 1) luminous flames; 2) molybdenum; 3) zirconium carbide; and 4) microstructured silicon coated with Au film. It has been shown that the thermal radiation of:

- a) Luminous flames in the case when $K_v L \ll 1$ and that of a black body radiation belong to the same universality class;
- b) Molybdenum belongs to the same universality class such as tantalum, tungsten;
- c) Zirconium, titanium, and hafnium carbides has a similar relationship between T and v_{max} . This means that they belong to the same universality class;
- d) Microstructured silicon coated with Au film has the same universality class as, for example, ZrB₂-SiC-based ultra-high temperature ceramic.

The proposed method, as well as the described materials in this chapter can be used by:

1. Lecturers conducting a course of thermodynamics and statistical physics on the topic related to the thermal radiation of a blackbody.
2. Students who conduct their own research for M.Sc and Ph.D. degree.
3. Professional scientists.
4. Private companies, and others.

ACKNOWLEDGMENTS

The authors cordially thank Professor L.A. Bulavin and Professor N. P. Malomuzh for fruitful discussion. Special thanks to Professor Guojin Feng for providing us with experimental data on the normal spectral emissivity of the microstructured silicon coated with Au film.

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Chapter 13

**PHYSICS OF BIOLOGICAL MEMBRANE:
AN INTERDISCIPLINARY APPROACH
TO RESEARCH AND EDUCATION**

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ABSTRACT

The study of the structural and dynamic processes occurring in biological membranes represents a central topic in many aspects of science. Those processes involve collective behavior of a great number of interacting molecules, while the understanding of the structure-function relationship require the simultaneous calculation (and simulation) of a large number of parameters. Self-assembly processes in biomembranes represent the cornerstone of the functioning of biological systems, due to the crucial role of the complex macromolecular assemblies containing proteins, nucleic acids, lipids and carbohydrates components. In this chapter, we illustrate some of the main approaches and techniques applied for the study of biological membranes and the multitude of processes occurring simultaneously in a wide range of the space-time domains. The future challenge in this research field must provide the integration of the different research/teaching models into a common background based on multi- and interdisciplinary approaches that combine the expertise coming from the different disciplines.

Keywords: biological membranes, biophysics, biotechnology, multidisciplinary teaching approaches

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1. INTRODUCTION

With the aim to prepare students and researchers for the study of modern biophysics, educators should provide frequent opportunities to investigate interdisciplinary scientific questions and problems. The development of interdisciplinary programs at the university level must include changes in curriculum, instruction, assessments, and teacher professional development in order to support conceptual understanding and establish cross-disciplinary connections [1-3].

The study of biological membranes represents a central topic at the crossroad of different disciplines including biochemistry, biotechnology, and nano-medicine.

The scientific investigation of biological membranes involves the collective behaviour of numerous interacting (macro-)molecules, while their complete structural description requires the simultaneous calculation (and simulation) of a large number of parameters [4]. The traditional bottom up approach for the study of bio-membranes involves investigations of processes that take place in a wide range of relevant distances and time scales. For these reasons the self-assembly properties of bio-membranes has been the object of intensive research both from the experimental and theoretical point of view, while the study of their structure-function relationship and their related dynamic processes represents a central topic in many branches of science [5-9].

In this respect, the challenge of planning future teaching and research programs with a central focus on biomembranes passes through the integration of the different scientific approaches and training intervention on a common background, in order to stimulate new discoveries and new ways of operating. To achieve this objective, the scientific research approaches need to improve the resolution of experiments, together with the improvement of the theoretical models and the computational efforts.

The integration efforts into a multi-scale description of the biological membranes systems require the integration of multi- and interdisciplinary approaches that combine results coming from a wide range of sub-disciplines, such as biophysics, biotechnology, cell- and molecular biology, physiology, bioinformatics and cybernetics.

2. THE STUDY OF BIOLOGICAL MEMBRANES: A CENTRAL TOPIC AT THE CROSSROAD OF DIFFERENT DISCIPLINES

In living systems the cellular plasma membrane represents a selectively permeable interface between the extracellular fluid environment and the internal cell cytoplasm. This protective barrier of the cell, which is mainly composed of lipids, proteins and sugars, is involved in many important cellular functions such as signalling and sensing, selective transport of matter, cell adhesion and electrical action potential propagation [10-12].

12]. In basic research, biomembranes are also important as delivery agents for drugs, enzymes and genetic material through the living cell membranes and other hydrophobic barriers of the bio-nanomaterials. For this reason the study of biological membranes represents a central topic at the crossroad of different disciplines including biochemistry, food industry, biotechnology and nano-medicine [13-16].

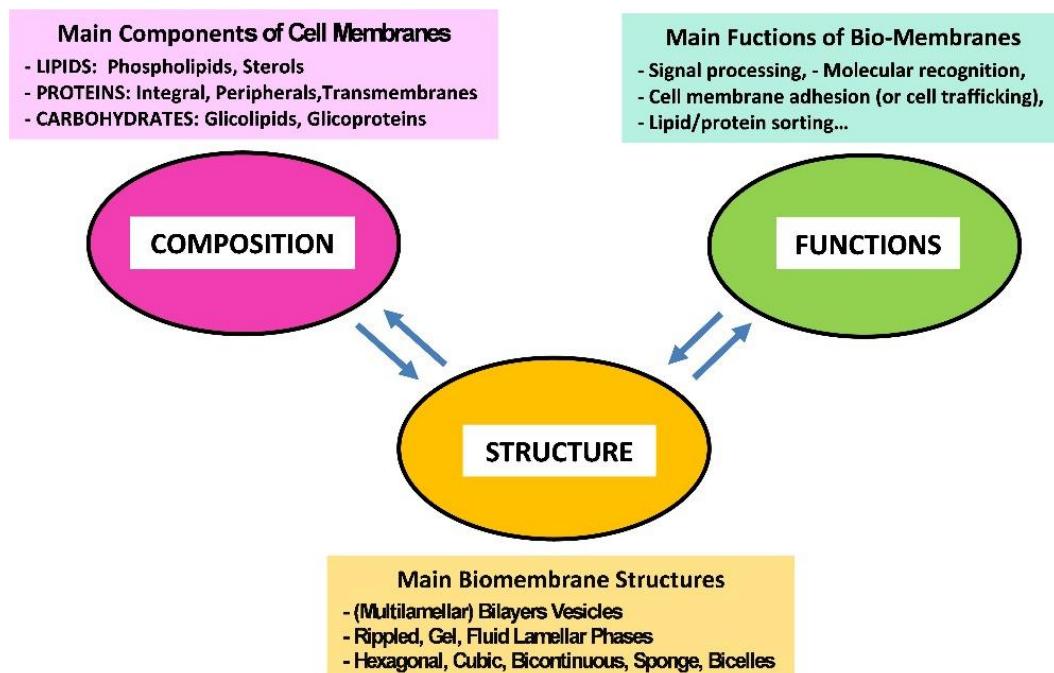


Figure 1. Schematic representation of the synergistic relationship between composition, structure and functions in a biological membrane system.

As reported in Figure 1, there is a synergistic relationships between the biomembrane's composition, structure and functions. The complex biomembrane's phase diagrams, which is rich of different structures and morphologies, require different strategies in order to elucidate the fundamental properties of the involved self-assembly processes as well as the underling molecular collective phenomena involved in the biological functions [17-21].

3. EXPERIMENTAL INVESTIGATION OF BIOMEMBRANES: A CONCEPTUAL FRAMEWORK IN TEACHING AND RESEARCH PROGRAMS

The current challenge of biomembranes research is to elucidate the molecular interactions and main components distribution (i.e., lipids, proteins and carbohydrates)

within the complex environment of the living organisms. This allows to establish the interconnection between composition and structure, and to extract the underlying organization principles that regulate the *biological functions*.

A conceptual framework of the experimental characterization approaches can be proposed for teaching and research purpose (see Figure 2). In this conceptual framework the experimental characterisation methods of biomembranes can be grouped into three main conceptual categories.

The first category focuses on the detailed analysis of biomembranes composition, which is attained by employing mainly the high-resolution mass spectroscopy techniques [22]. Detailed information about the profile of the liposome's population is also obtained by means of the size-exclusion chromatography (SEC) technique [23]. This technique is able to separate and quantify liposome populations by exploiting the time-based resolution of hydrodynamic size, where the separation process is based on the elution velocity from a column equipped with a porous substrate.

The second category of characterisation methods focuses on the structural investigation of biomembranes by means of in vitro experiments. Among the experimental methods used, the Neutron and X-rays small angle scattering (SANS and SAXS) and diffraction approaches represent probably the most important non-destructive experimental techniques for the structural investigation of bio-membranes in complex biological systems [24-28]. Those techniques efficiently evidence the formation of different structures and topologies thus highlighting the important role of the relevant molecular conformations in many different processes of life science [29-33]. Those techniques, that include the structural biology approach, can be complemented with nuclear magnetic resonance (NMR) or (cryo-)electron-microscopy (EM) experiments that provide detailed insights into lipid bilayer packing and phase states, protein conformations and folding, and sugars inclusion [34, 35].

Many other analytical methods have been employed with the aim of determining the affinity of compounds for biomembranes, including the spectroscopy techniques such as FT- infrared (IR), ultraviolet (UV), electron spin resonance (ESR), electron paramagnetic resonance (EPR), circular dichroism, in connection with complementary biophysical techniques, such as the differential scanning calorimetry (DSC), isothermal titration calorimetry (ITC), surface pressure changes and potentiometric measurements [4, 10, 11].

Finally, the third category focuses on the characterisation of biomembrane's functions within the complex environment of living cells. In this case the *optical far-field microscopy* is usually the method of choice, since it allows observation of structures and dynamics in an almost non-invasive manner. Specificity is achieved by fluorescence labeling of the molecule of interest. The full potential of far-field fluorescence microscopy is limited by constraints in spatial resolution (limited by diffraction to about 200 nm for visible light) and temporal resolution (limited by the speed of the image recording). [36]. Recent instrumental progresses enhanced the resolution of optical

microscopy, thus allowing to approach the molecular scale details of the living cells by means of fluorescence correlation spectroscopy (FCS), enabling the observation, in a non-invasive way, of the molecular diffusion and interaction dynamics with millisecond time resolution [36].

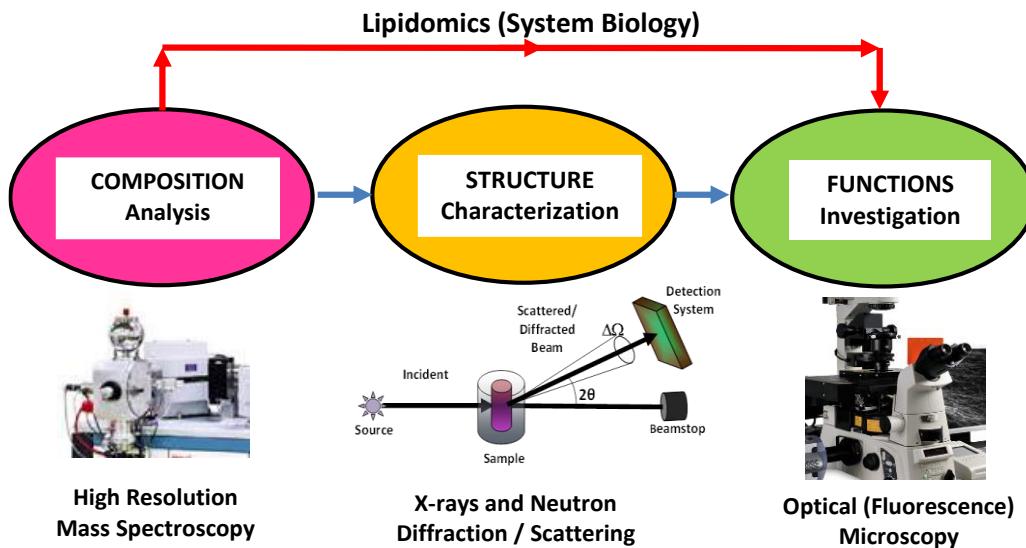


Figure 2. A conceptual framework of the main experimental techniques for the study of biomembranes.

Finally, it is worth pointing the importance of the interactions in the control of intermolecular self-assembly processes in complex multicomponent structures of biomembranes systems. The complex behaviour, in fact, is due to the simultaneous presence of both polar and apolar moieties within the architecture of the bio-molecules. This simple structural features dictates their intermolecular self-assembly through the delicate equilibrium of several possible interactions: polar–polar, polar–apolar and apolar–apolar forces, eventual directional H-bonds, steric hindrance and hydrophobic effects [37-39]. All those interactions allow the building up of the biomembrane's structure.

The strength of all these interactions determines the local aggregation state at room temperature (ordered, disordered, liquid-crystal) and their aggregation pattern (lamellar, bilayer, hexagonal phases). The combination of all these interactions determines also the formation of energetic barriers controlling the thermally activated diffusional and rotational molecular dynamics and, therefore, the time scale of the local position and orientation order of the single building-block molecules within the biomembrane's aggregates [40-42].

It turns out that the peculiar dynamical processes observed in biomembranes assemblies is the result of a rich scenario of possible inter-molecular interactions which allow the formation of supramolecular structures at different levels of complexity in a

manner similar to other relevant complex nanostructured systems encountered in material science and biotechnology [43-46].

4. OVERCOME THE SPACE-TIME RESOLUTION LIMITS OF EXPERIMENTS: THE MOLECULAR DYNAMIC APPROACH AND THEORETICAL METHODS

As bio-membranes functions emerge at different hierarchical levels (multi-scale systems) across a wide ranges of space and time domains, the bottom up approach of cell membranes (i.e., from molecules to cells) requires detailed information over the complete space-time range (from fast to slow and from small to large). Even though a considerable progress has been made with the experimental investigations of biomembrane structure and dynamics, the investigation of relevant self-assembly mechanisms is still limited by the space-time resolution of the experimental methods, such as the optical (fluorescence) microscopy and the complementary spectroscopic techniques. In this respect, the progress of molecular dynamics (MD) simulations methods offers the opportunity to overcome those current limitations, allowing the study of collective behavior of multicomponent systems in great space-time resolution [47, 48].

Molecular dynamics (MD) simulations methods are able to describe a wide range of biophysical processes, addressing a variety of interdisciplinary issues including conformations of biomembranes, proteins, relevant bio-conjugates and biomaterial complexes [48, 49]. Moreover, the MD approach has proved particularly interesting for the study of self-assembly processes of nanoparticles and their interaction with biological systems, like carbohydrates, proteins, biomembranes and cells.

An increasing number of investigations with MD simulation, have been recently partnered with experimental methods [49-52], as computer simulations approach can track the system complex behaviour across a vast space-time scales ranges, otherwise inaccessible with traditional experiments. This comes at the cost of the simulated system dimension (i.e., limited to thousands of molecules) and only for short time periods (microseconds). Moreover MD resolution is limited to reveal only fast and nanoscopic processes instead of slow and large biophysics processes usually accessible by optical microscopy. To overcome this problem and extend the spatiotemporal scale of MD-simulation, different methods have been developed (such as the “coarse grain”) without sacrificing too much the molecular details of the approximated model system [53-55].

The study of the structural behaviour and structure-function relationship in complex multicomponent systems of biophysical interest can also be addressed by investigating suitable theoretical models that make use of the concepts of the statistical physics and thermodynamic approaches. Among them, the mean-field approximation (MFA) [55] and

the Ornstein-Zernike (O. Z.) integral equation approach [56, 57] are widely employed in the field of biotechnology and nano-medicine. Those approaches has been employed to study the range and strength of a large variety of soft interactions [58-60] usually encountered in biological systems, including nanostructured colloids [61-64], amphiphiles [65-67], proteins [68-69], dendrimers [70-73], hybrid and polymers-based nanocarriers [74-78], and model biomembranes [79-83].

5. A MODERN INTERDISCIPLINARY FRAMEWORK FOR THE STUDY OF BIOMEMBRANES: SYSTEM BIOLOGY AND THE LIPODOMIC APPROACH

An interesting example of the interdisciplinary approach in life science is given by the *systems biology* method. This approach is based on the collection of information and data from many components in parallel, using the so called “-omics” technologies, like metabolomics, proteomics, genomics [84]. Systems biology has grown as an interdisciplinary approach of many previous fields, such as biophysics and biotechnology, cell- and molecular biology, physiology, theoretical biology, nonlinear dynamics, bioinformatics, systems theory and cybernetics.

This approach aims to understand the complex interactions and functioning of the living cell at various levels, by inferring the complex pathways and intermediaries that govern each biological (physiological or pathological) process. From a conceptual and operational point of view, the approach aims to transform molecular biology from a reductionist, hypothesis-driven, experimental method into an holistic data-driven field of research.

As lipid bilayers membranes represent one of the main components of biological membranes, the *lipidomics* research field emerged as an important subfield of system biology method for the study of biological systems at an interdisciplinary level [85]. Lipidomics, is the study of pathways and networks of cellular lipids that attempt a large-scale mapping of the complete cellular lipid species (lipid profile) within a variety of biological systems (such as a cell, tissue, or organism). Dynamics profiles of cellular lipids and the changes that occur after the perturbation of the system (cell), are examined in order to identify biomarkers and elucidate the main changes in its physiological or pathological state.

As lipids play an important role in many metabolic diseases such as diabetes, obesity, atherosclerosis and hypertension, the lipidomics approach is considered as a subset of the more general field of “metabolomics” which includes three other major classes of biological molecules (proteins/amino-acids, sugars and nucleic acids). Lipids bilayers

biomembranes also regulate protein functions and gene transcription, and for this reasons they are also considered as a part of a dynamic “interactome” within the cell.

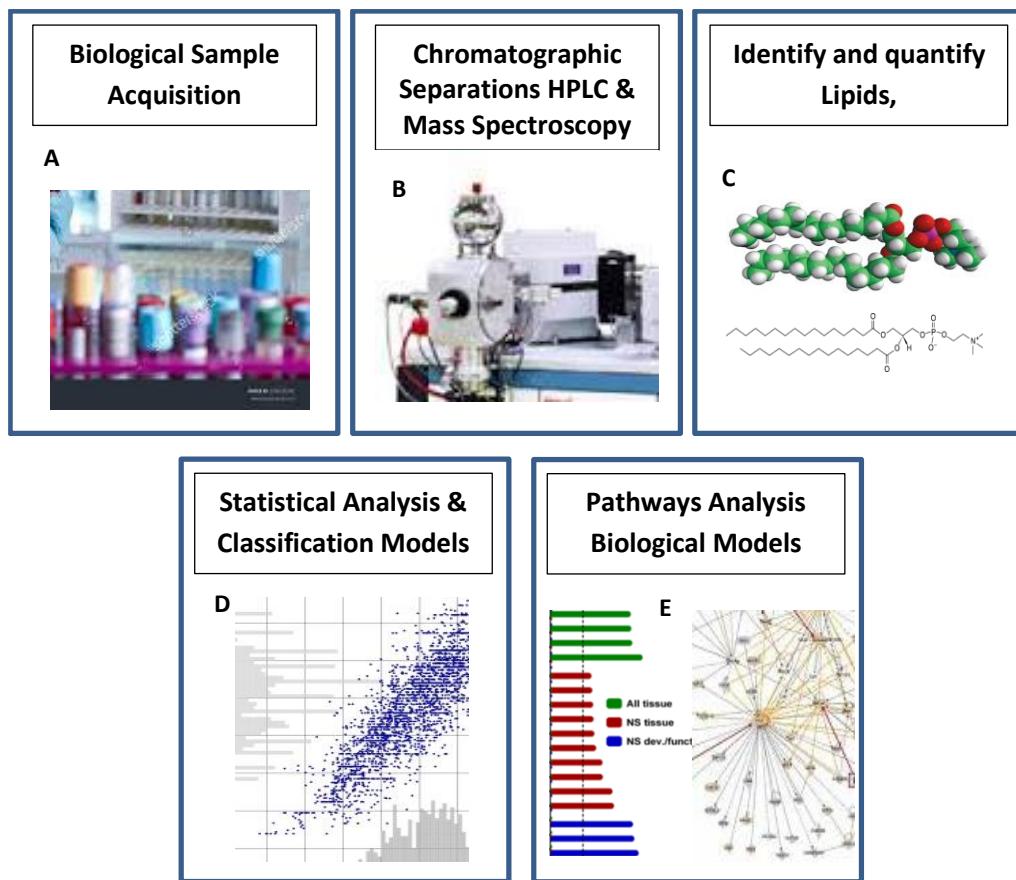


Figure 3. Sketch of the lipidomic workflow. A sample of a biological systems (cell, tissue, or organism) (A), is analysed by means of a chromatographic separations (HPLC) instrument connected to a high resolution mass spectrometer (B) in order to identify/quantify the lipid profiles (C) relevant to a specific biological (or pathological) condition. The large-scale mapping together with suitable statistical analysis and classification models (D), allow to a pathway and networks analysis to identify the relevant biomarkers associated (E).

Those rapidly expanding fields complements the huge progress made in proteomics and genomics (so called *omics-technologies*), all of which constitute the family of systems biology [84]. Introduction of the lipidomic approach in dedicated teaching and research programs, allow a systematic study of the biochemical mechanisms of lipid-related disease processes through the identification of the alterations in cellular lipid metabolism, trafficking and homeostasis. This novel conceptual organization of disciplines facilitates the framing of the study of biomembrane within a true interdisciplinary approach at the crossroad between chemistry, informatics, mathematics, biology and medicine.

6. STRENGTHENING THE MULTI- AND INTERDISCIPLINARY ASPECT OF BIOMEMBRANES STUDY

As the molecular level investigation of bio-membranes involves the collective behaviour of numerous interacting (macro-)molecules, their complete structural description requires the simultaneous calculation (and simulation) of a large number of parameters due to the variety of the interactions involved and the number of conformations which are present [86-89].

The traditional bottom up approach for the study of bio-membranes involves the investigation of relevant nanostructured systems starting from the analysis of molecular interactions (~10 nm), to the assemblies of lipid-protein complexes (~100 nm) up to the meso-scale (~1 μm) and macro-scale (tissues and cells). This means that the bottom up approach request the investigations of the structural and dynamic processes over a wide range of distances and relevant time scales.

Biological membranes in living organisms, which have the prominent role of tissues and cells protection from foreign molecules, play also other essential functions in living systems. For example they allow the exchange of information between extra- and intracellular environments due to its biochemical-active surface, that include amount of associated enzymes, ion channels, receptors and signaling molecules.

Finally, supramolecular structures of biomembranes also have a crucial role in cellular homeostasis, metabolism, growth, and even cellular death. Therefore, study of the alterations in the structure/functions relationship of relevant biological membranes are crucial for the understanding of the pathological effects which are at the origin of many diseases.

As the natural cell membranes present a great complexity of structures, with a large variety of cross-connections and functionality, the study of simplified (artificial) model systems, greatly helps the scientists to understand the effects of membrane lipids in drug transport and uptake into cells, and their possible toxicity effects. Using artificial nanostructured materials as simplified models for the study of cell membranes processes has given a strong input to the understanding of the complex interactions that a biomolecule can develop toward biological membranes [90-93].

Moreover, the specific dynamical processes observed in a biological membrane and in bio-nanostructured assemblies depend on a rich scenario of multicomponent intermolecular interactions which allows the formation of supramolecular structures at different levels of complexity in a manner similar to other complex nanostructured systems of biotechnology and materialscience [94-97].

Finally, the study of the molecular events occurring on cell membranes, as well as the multiplicity of interactions that involve bioactive compounds (in either physiological or pathological situations) requests then an interdisciplinary effort of many different field of

science (see Figure 4). A novel conceptual framework towards an interdisciplinary approach is therefore of paramount importance, to enlarge our knowledge of many diseases and to identify further potential therapeutic targets.

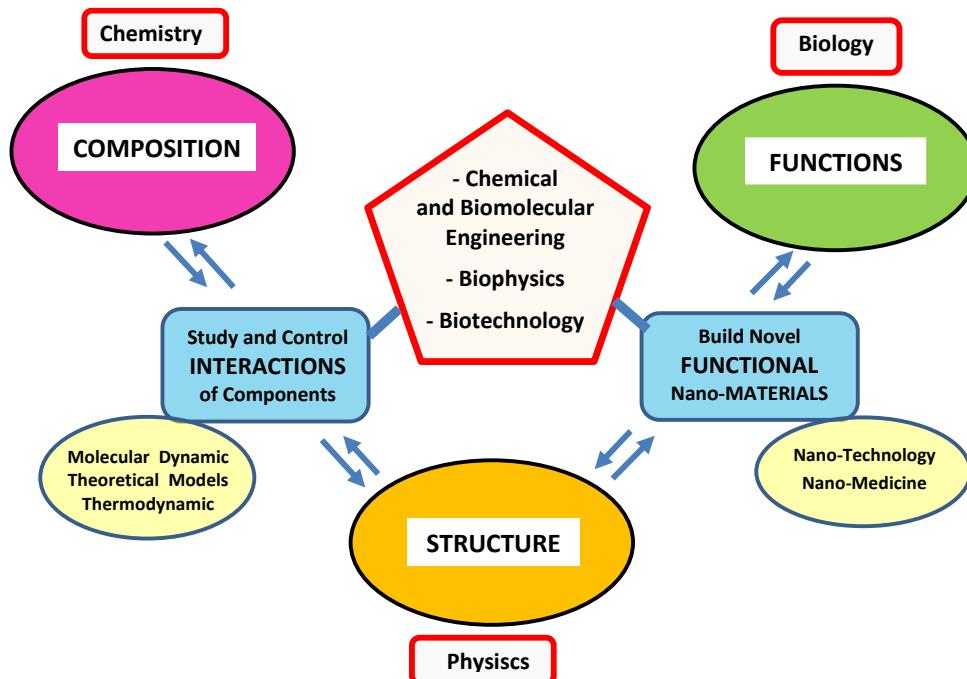


Figure 4. A conceptual description of the main disciplines involved in the interdisciplinary study of biological membranes.

CONCLUSION

The study of biological membranes represent a central topic at the crossroad of different disciplines including biochemistry, biotechnology, and nano-medicine. The scientific investigation of biological membranes involves the collective behaviour of numerous interacting (macro-)molecules, while their complete structural description requires the simultaneous calculation (and simulation) of a large number of parameters. The future challenge must provide an efficient integration of the different teaching approaches and research models into a common background, in order to stimulate new discoveries and new ways of operating.

To achieve this objective, we need to improve the resolution of experimental approaches, together with the improvement of the theoretical models and computational efforts, and integrate them into a multi-scale description of the biological membranes systems. This effort require an integration of multi- and interdisciplinary approaches that combine results coming from a wide range of sub-disciplines.

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