Part I

Designing Complex (Meta)Materials: Results and Perspectives

1 Metamaterials: What Is Out There and What Is about to Come

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1.1 Technology and Science: A Two-way Interaction

Developing[1] *new science produces technological benefits*: this is so often repeated it is a commonplace nowadays. In our opinion the converse statement, i.e. that cutting-edge technology provides substantial stimuli for scientific innovation, has not to be underestimated either. Hence, the interaction between science and technology has not to be regarded as unilateral/one-way. In fact (as summarized in Fig. 1.1), the investigation of theoretical models describing some known phenomena can lead to the development of new *scientifically designed* devices which, in turn, might unveil some not-yet-discovered phenomena. This process of scientific modeling, designing and experimental discoveries could in principle keep going indefinitely. Of note, the process leads to the discovery of progressively "higher order" phenomena, which become accessible only after some necessary "lower order" modeling and discoveries. Apparent examples of very high-order phenomena are easily found in current research (to mention a recent and widely known case) in quantum gravity, concerning the discovery of gravitational waves.

It is a matter of fact that emerging technologies and development of the exact sciences have a close relation. Actually, it is a *leitmotiv* in the History of Science that new technological possibilities lead to new phenomenological evidences, putting in crisis any existing paradigm and gradually leading to a totally new one. The birth of scientific technology in the Hellenistic World, the rise of modern mechanics in the age of Galileo, and the development of thermodynamics in the early nineteenth century are relevant examples of this phenomenon. In all these cases, it is by now well-established among historians of science that a significant conceptual revolution occurred driven by technological reasons. The main goal of these successful new ideas, that nowadays after a long and troublesome process we call *classical physics*, was to design and describe new technology (as for example bombards, steam engines, or catapults). Let us examine in more detail one of the above-mentioned examples: the revolution in the conception of mechanics due to the results of Galileo and his school. Simplifying necessarily a complex matter, we can say that, while within the Peripatetic school (the philosophic tradition based on Aristotle) the motion of objects like the projectiles of bombards does not obey the same laws that govern celestial mechanics. Galileo managed to include phenomena

[1] The present Introduction is based, with large additions and significant updating, on the papers [1, 2].

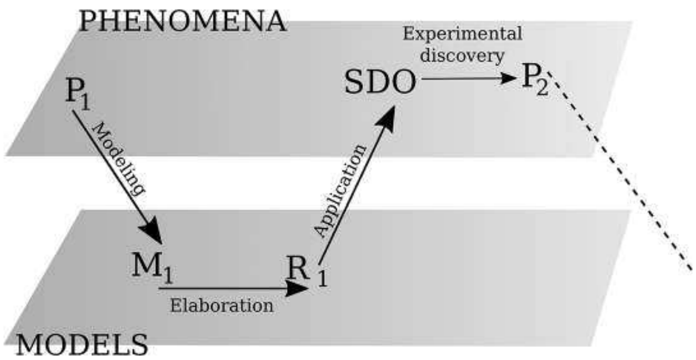

Figure 1.1 A graphical representation of the two-way interaction between science and technology in time. A phenomenon (P_1) appears which is not yet scientifically described; a theoretical model (M_1) is built; theoretical results (R_1) come from the study of (M_1); the application of (R_1) leads to a *Scientifically Designed Object* (SDO); a new phenomenon (P_2) is discovered as a byproduct of (SDO).

which were previously deemed to be completely separate (i.e. those characterising the Celestial World and the Terrestrial World) in the same conceptual framework. Therefore, he established the fundamental uniqueness of Nature regarding its division in Celestial and Terrestrial World, and concerning the latter in natural and man-made objects [3].

In our opinion, the new technological possibilities in controlling the micro- and nanoscale of materials, which are capable of producing objects that, at the macro-level, display properties that are not found (or very rarely found) in nature, are leading mechanics to a similar conceptual revolution. Indeed, these methods often produce objects with peculiar behaviors that cannot be explained by using the classical point of view and therefore new theoretical models have to be developed.

Moreover, due to the technical manufacturing advancements experienced in the last years, we are forced to consider again the whole relation between theoretical (and applied) mechanics and technology. Indeed, thanks to advancement of manufacturing processes it is now possible to design and develop materials, the so-called metamaterials, with properties that cannot be found directly in nature, while for thousand of years these properties have been considered as something which existed but could not be exploited. Several scientific questions which demand an answer are now arising due to the advancement of techniques like electrospinning, self-assembly and 3D printing. We are living today, as in the history of science sometimes happens, in an historical moment in which the scientific modeling is behind the technological advancement. The multi-scale (and multi-physics) description of such materials shows a wide range of exotic behaviors which hides, in their inner organization, a high level of complexity. Therefore, an effort in the development of mechanics and physics of solids and fluids, of computer-aided technology, and of mathematical and numerical modeling is now required. The challenge of design and construction of metamaterials is calling for a stronger theoretical foundation and a pragmatic understanding of what is feasible today.

1.2 The Importance of a Universal Terminology

A common feature of novel research topics and emerging fields is the lack of a general order based on well-established language and concepts. The main problem to which a confused terminology gives rise is the creation of barriers complicating scientific communication between researcher from different topics, which is a serious problem in every branch of modern science. The research on design and manufacturing of metamaterials precisely exemplifies this phenomenon.

We incidentally recall that (modern) scientific biology started with establishing some precise taxonomy criteria (eventually to be updated according to our genetic knowledge) which unequivocally determine the scientific name of each species (once discovered). Although Aristotle (*De Partibus Animalium*) had already started such systematization of biological knowledge, it is only with Linnaeus (*Systema Naturae*, 1758, 10th edition) that taxonomical classification displayed its full descriptive power.

It is generally accepted that every part of hard science (including of course mechanics) should have at least the same level of exactness of biological taxonomy in its terminology. Actually, since hard science deals with a theoretical universe in which there are virtually infinite objects susceptible of meaningful definitions, this requirement is even more strict here than when studying sets of objects which are in principle finite (as biology does).

One of the frontiers of research in mechanics must be situated at the border separating the models introduced for describing "standard materials" and those for "exotic materials." There are many difficulties in recognizing where such a frontier is located, especially because the adjectives "standard" and "exotic" are very difficult to make precise. In what follows, we will consider as "exotic material" a system constituted at micro level by matter distributed in a refined and complex microstructure where, for instance, micro gaps divide different deformable micro parts which in some cases may undergo large localized micro relative displacement. With respect to this definition, a critical reader may even start discussing initially the most fundamental concept of "material" and the difficulties involving in its definition. Indeed, if there is a material at all in such a system one has to find it at the micro level, that is at the level in which the characteristic length is a fraction of the dimensions of the elements of the microstructure. To this reader, another one, even more critical, may object that, by magnifying the image further another microstructure may appear: this microstructure is constituted, for example, by the partially melted and partially agglomerated grains of the polyamide powder which has been used as initial input of the 3D printing process used to produce the considered specimens. These critical remarks, in different contexts and in different situations, have often been repeated to try to understand the ultimate nature of physical phenomena (see e.g. Democritus [4–6]).

Therefore, in an effort to be precise, we shall use the term *homogeneous material* as follows:

We assume that it is possible to choose a length scale L and a corresponding Representative Elementary Volume (REV) (a cubic volume whose sides are L) such that, by moving the REV in the specimen the overall (macro) mechanical response of the material included in it does not change and can be described exclusively in terms of overall (macro) kinematical descriptors which can be assumed to be constant for every REV.

A polyamide, when considering a REV including a group of grains, is a material in the sense of the previous definition. A pantographic sheet (that we will discuss in detail in following sections), when considering a REV including a group of cells is another material, although it consists ultimately, at a lower length scale, of another material, i.e. polyamide. We refrain here from any other philosophical consideration, which may cause us to go back to Heraclitus and Democritus, to discuss Epicureans and Boltzmann, ending with modern Truesdellism (see for more details e.g. [7, 8]).

After having specified what we mean by the concept of material, we observe that also the standard definition of "metamaterial" as given for instance by the statement (reformulating the corresponding entry of Wikipedia as read on 6 Dec. 2017) can be discussed:

> Metamaterials (a combination of the Greek word $\mu\epsilon\tau\acute{\alpha}$, meaning "beyond" and the Latin word *materialis*) are materials engineered to have property that is not found in nature. They are made from assemblies of multiple elements fashioned from materials such as metals or plastics. The constituting materials are *usually [our italic]* arranged in repeating patterns, at scales that are smaller than the wavelengths of the phenomena they influence. Metamaterials derive their property not from the properties of the base materials, but from their newly designed structures.

It is also clearly not fully correct. We are particularly surprised by:

- the occurrence of the adverb *usually*,
- the final statement which seems to underestimate the possibility to design very interesting metamaterials by considering many base materials which can show large differences in physical properties,
- by the obscure use of the expression "in nature."

Indeed, nobody can claim that either iron or stainless steel is a natural material. Humans needed many thousands of years to develop such "artificial" materials. However, nobody designates them "metamaterials." We would like to avoid considering something as "natural" simply because we are accustomed to its use and its existence.

Tentatively we propose here to call *metamaterial*:

> *A material which has been designed to meet a specific purpose, by combining more elementary materials (characterized by a smaller micro length scale) and by shaping them with geometrical structures and mechanical interactions (what we call a* ***microstructure****) characterized by the same micro length scale.*

We will call *micro* the level at which the considered structure shows all its (geometrical and mechanical) inhomogeneity and complexity and call *macro* the level where it behaves as a homogeneous material.

Note (see [9, 10]) that the more interesting cases, i.e. the cases in which the macro metamaterial shows a completely different behavior when compared with the micro behavior, is represented by micro structures in which an extremely marked contrast of mechanical and geometrical properties occurs.

One of the main goals of this introduction is to show how different research fields are addressing, by means of several approaches and maybe not in an obvious way, different points of view of the same general problem. At the same time, we want to provide a reasonable (of course far from being exhaustive) coverage of the relevant literature.

In the current research in applied mechanics, what we call here metamaterials, according to the previous definition, have been labeled as:

- **Metamaterials** [11–15],
- **Multi-scale Materials** [16–19],
- **Multi-physics Materials** [20–34],
- **Complex Materials** [35–41]
- **Architectured Materials** [42–45, 45–48],
- **Optimized Materials** [49–51],
- **Negative Mechanical Constitutive Coefficients Materials** (Poisson ratio, modulus, stiffness, etc.) [52–56]
- **Smart Materials** [57–61],
- **Advanced Materials** [62–65],
- **Composite Materials** [66–70]).

As for the theoretical aspects, we may find, for example:

- **Generalized Continua** [71–79],
- **Higher Gradient Continua** [80–87],
- **Continua with Microstrains** [88, 89]
- **Cosserat Continua** [90–97],
- **Micro-structured Continua** [98–114],
- **Micropolar Continua** [115–118].

Apart from some cases of almost exact equivalence (the identification of the overlapping between some of the previous fields are studied in some dedicated work, we refer to [4, 74, 119–124]) these labels do not exactly refer to the same scientific content. Rather, what they share are goals and *motivations* behind their origins.

The real challenge, in the opinion of the authors, for both applied and theoretical mechanics can be summarized in the following:

MISSION STATEMENT – to choose the governing equations of a material describing its desired behaviour, and successively to design and produce a complex micro-structure (or a multi-physics system) whose behavior is suitably described by the chosen equations.

This mission statement is the common foundation of all the research lines indicated by the previous labels. This point of view, in our opinion, may provide a useful guide in this spectrum of complicated problems. Indeed, by keeping clear this final aim we do not distract attention from the useful scientific content by focusing on cumbersome technicalities and subtleties. Thus we simplify the transfer of information about tools and methods from different areas of science, providing us with a stronger arsenal for dealing with the challenges.

The authors dare to share the opinion of Richard Toupin (private communication at *4th Canadian Conference on Nonlinear Solid Mechanics*, Montreal, 2012) about the reasons behind the dangerous proliferation of names for the same physical or mathematical concepts. While referring to a famous quote by Poincaré,[2] Toupin declared that often mechanicians, simply to distinguish themselves among others and in order to have more chances of financial support, rename "clouds" of concepts, collected in existing literature, with new terminology. Of course, Toupin blamed this attitude, considering it detrimental for the advancement of knowledge [2].

1.3 The Relation between Mechanics' Fundamental Hypotheses and Existing Technology

The technologies of every advanced society have been based on mathematical modeling capabilities [125]. The Archimidean mathematical description of engineering artifacts and phenomena characterized the Western civilization. The great technological and economical development of the Age of Enlightenment was based on solid mathematical foundations. However, in this period, and in particular in the following Industrial Revolution, engineering was based on the limiting (but simplifying) assumption that mathematical modeling merely had to be focused on the description of pre-existing materials in order to allow selection of materials in structural design (an introduction to material selection can be found in [126]). Of course, this idea and the hypothesis assumed by the fathers of engineering science as it is known today (Poisson, Navier, Cauchy, Piola, Maxwell, etc.) was based on the observation of (natural) phenomenology, but the whole scientific and technological thought founded on this paradigm became basic doctrine. Indeed, in the mind of engineers and scientists, it was deeply established.

As we have already mentioned, however, "higher order" phenomena, discovered by means of technological innovation, cannot be neglected without limiting our scientific prospects. In fact, several interesting investigations have seen their evolution stopped precisely because of the automatic (and erroneous) distinction between natural phenomena and phenomenological reality *tout-court*, even if the brand-new technology of computer-aided manufacturing has made this distinction completely outdated (see [127]).

To give our reasoning a more concrete character, let us consider a specific example, concerning the concept of external contact action. If we deal with deformation energy depending on the objective part of the first gradient of the displacement field, i.e. if we consider classical Cauchy continua, we are essentially limiting external contact actions only to surface forces. However, complex microstructures may give rise, in their homogenized limit, to models based on higher gradients (see above in the previous section) which are able to describe also other possible external contact actions, such as double forces, line forces, concentrated forces and higher order objects [128]. In other words, since 3D printing, electrospinning, or other kinds of technical possibility allow you to manufacture objects and materials whose microstructures in a continuum limit can sustain higher order forces (for instance, double forces), the theoretical model that we are considering cannot neglect them any more. Therefore, to enrich the set of

[2] "*Mathematics is the art of giving different things the same name*."

behaviors that your theoretical model can describe, you have to reconsider its assumptions. This is what the title of the present section aims to mean: the most appropriate set of assumptions for the theoretical mechanical construction (and in fact, for science in general) has to be determined by the technological possibilities. Therefore, during the formulation of the theoretical model it is not sufficient to consider only purely abstract reasons without including in the picture also the effects of novel technologies – a notable example where the description of unusual response of materials to elastic waves required an appropriate extension of elementary dynamics' concepts can be found in [129].

One of the most recent conceptual revolutions caused by the emergence of new technology happened around 1940 due to the development of the first prototypes of digital computers based on Turing–von Neumann machines. In particular, the possibility to compute solutions to complex partial or ordinary differential equations for the design of large-scale production [130] and for scientific experiments [131] by using digital machines became concrete. Since people working in engineering and science could not wait for the final establishment of the superiority of digital computers, the supporters of analog computing, inspired by the new paradigm, started to synthesize analogous electric circuits described by different mathematical equations. The aforementioned mission statement has several methodological analogies with this example. Indeed also in this case, once the equations governing the desired macroscopic behavior of the material have been chosen, its microstructure (or a complex multi-physics system) has to be synthesized, giving rise to the behavior described by the chosen equations. However, the main difference between the competition between analog and digital computers (that was historically important in the development of computing) and the case of metamaterials is the wider generality of the latter in the relevant applications and systems and which therefore gives rise to demands for a greater effort and sophistication in theoretical tools.

1.4 Three Approaches to Accomplish the Objective

The beginning of material technology can be traced back to non-sapiens hominids. This audacious journey can be summarized in the following basic steps [44]:

1. the on site available materials (e.g. bone, wood, or native metals) were used;
2. the optimization of particular kind of materials (e.g. empirical metallurgy techniques) based on empirical attempts started;
3. the birth of approaches based on science (e.g. scientific metallurgy and later the study of polymers, etc.) occurred;
4. the so-called *hyperchoice of materials*. Here we mean the development of scientific tools and methods in order to select and compare different classes of materials which, individually considered, had already optimized applications in the engineering science;
5. study of the multi-functionality of materials, with increasingly ambitious requirements for materials capable of fulfilling conflicting needs.

Of course, mathematical modeling plays an increasingly important role passing from one step to another and today the available theoretical tools are not enough to fulfill the multi-functionality requirements coming from technical possibilities and industry [42, 132].

In the following subsections we will outline three possible ways to achieve the mission statement.

1.4.1 Trial and Error

In this approach a conjecture on the structure of a system exhibiting a given behavior is based on experience and on physical intuition. The validity of such a conjecture has then to be proved by means of experimental evidence on prototypes. Of course, numerical simulations, in this approach, play a fundamental role in orienting the trial conjectures toward the right one. Among the powerful methods available today, Finite Element Analysis allows us to rapidly get information on the main quantitative properties of complex mechanical systems. Indeed, its flexibility allows an effective description of the complex geometry of systems like metamaterials (recent applications can be found in [133–137], while an historical reference is [138]). Some interesting applications are the modeling of fracture phenomena by using finite elements with particular interfaces (see for instance [139, 140]) and isogeometric analysis (see e.g. [141–147]) performed by introducing elements with high regularity properties.

Another powerful computational tool is the so-called Molecular Dynamics that is particularly feasible to numerically study systems consisting of a huge number of particles. It employs equations of motion of classical mechanics to numerically compute the trajectories of N particles in the phase-space, i.e. the $6N$-dimensional space of positions and momenta (see e.g. [148] for an introduction). Finally, computational methods based on scale-bridging like DDD, QC, CADD, MADD (see [149] for a discussion by means of an example of the comparison of these models and other general problems) which were initially developed to describe small-scale systems in terms of classical physics, can be useful to describe inelastic mechanical systems.

1.4.2 Generalized Continua Models

The previous approach is the most suitable when only a simple refining is needed after the achievement of major advancements. However, this is not the most general scenario and, if we want to achieve technological progress by means of completely new concepts, we may need to consider a drastic change of paradigm by reconsidering a considerable part of engineering science. An effective way to achieve this end may be to re-examine a research line started by Gabrio Piola [150] about the foundation of continuum mechanics. Actually, maybe even in an unconscious way, a revival of the ideas of Piola has already started and one of the most fruitful examples is the field of Peridynamics (for an historical perspectives see [4], while relevant results may be found in [151–155]). Basically, Peridynamics is the modern term for the most general formulation of continuum mechanics initiated by Piola, initially introduced to describe