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A Tutorial on Mathematical Models in Materials Science

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> *"The most incomprehensible thing about this universe is that it is comprehensible"*
>
> ***Albert Einstein***

Abstract: Materials Science (*MS)* broadly concerns with the nature, properties, and use of materials. It accompanies mankind from the very beginning of its existence. The *MS* investigates the effect of the structure in various scales on materials properties. Mathematical Models (*M&M*) is a routine part of materials science research and development. It is appropriate to understand how and if modelling differs from ordinary quantitative science and to assess the successes and failures of the methods. *M&M* plays a key role in ensuring the success of innovative systems, which meet existing needs or introduce new standards, by disrupting the status quo. The subject is now sufficiently mature to bear some constructive self-criticism and exaggerated claims. The paper discusses various aspects of *M&M* and outcomes are intended to be generic, although the examples used come from the various aspects of metals.

Keywords: Idea, product, model, modelling, validation, material properties, and development

1 Introduction

Recently, the term "materials science" aka *MS* is used primarily to denote empirical study, fundamental research, synthesis, and its productions. *MS* area is great significance in solid-state physics areas, which focuses on the physical properties of solid materials. The term MS is a broader context, which involves interdisciplinary interactions among mathematicians, physicists, scientists, engineers, chemists, biologists and so on. A fundamental objective of theoretical work in materials science is the description of properties of bulk materials based only on the properties of and interactions between their constituents. During the last 40 years, tremendous progress has been made toward this goal of understanding and predicting material properties from such a microscopic viewpoint. *MS* appeared as an independent branch of science, which was created at the beginning of industrial revolution, and in consequence to the materials science. It is a challenging endeavour to trace the properties and the development of materials in the light of the history of civilization. The interaction between the *MS* and mathematical models (*M&M*) increases due to the physicists, material scientists, and mathematical researchers. *M&M* has become as much a part of materials science as experimental characterisation for two reasons. First, to compete, industry must achieve solutions using minimal resources. Second, scientists are excited by the quantitative expression of multivariate problems.

Involvement of government initiative are critical to the success of industries such as the aerospace, automotive, biomaterials, chemical, electronics, energy, metals, and telecommunications industries. The purpose of this paper focuses on directions for potentially promising collaboration between materials scientists and mathematical modellers. In view of the above, the paper discuss various aspects *M&M* in material science and so on.

A Complex System Needs Models: Generally speaking, engineers and scientists try to understand, develop, or optimize “systems”. A “system” refers to the object of interest, which can be a part of nature or a designed system or an artificial technological system.

2. Mathematical Models: Why, What and How?

2.1 Principles of MM

What is a *M&M*? What types of models do exist? Which model is appropriate for a particular problem? How does one set up an M&M? What are simulation, parameter estimation, verification and validation? A model is a representation of reality. Simply it is a simplification or abstraction. A model may be a physical representation. An *M&M* differs from the more tangible physical model, in that “*reality*” is represented by an equation or series of equations. The time and cost factors spent for an experimental seems proportional to the complexity and urgency of the systems. A *real-time* system is one which must respond to external changes within certain timing constraints. Observations and assumptions concerning the behaviour of real-time systems are explicit and objective. Therefore: “An inherent limitation of models is that judgments are necessary in building them”.

A prototype, an operational instance of the model, is used to evaluate the safety as well as the response of users to first-hand experience with the product concept, Figure 1. Due to invest of the state-of-the art additive manufacturing technologies *M&M* are proving to be a powerful tool for enabling the rapid construction of prototypes with minimal delays and costs. The impotent notion *dependability* encompasses several related attributes, such as availability, reliability, durability, safety, security, integrity, maintainability and so on.

In general, research activities in real-time systems have focused on scheduling or real-time tasks in systems that have periodic or aperiodic request patterns, multiple (interchangeable) computational resources, tasks of varying priorities, and real-time communication.

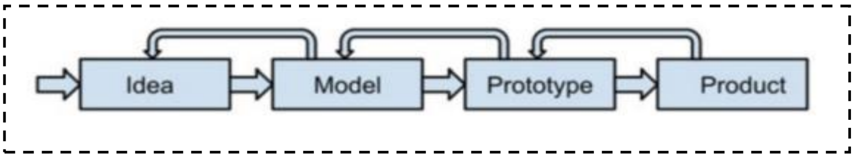


Fig. 1: A typical process for developing a new product

The formulation of a problem of *M&M* an object leads to a precise plan of actions. It can be conditionally split into three stages: model - algorithm - code (Figure 2).

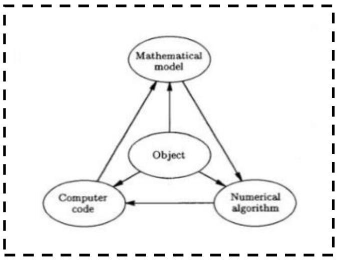


Fig. 2: Three stages of an Object

The methodology of *M&M* is the art of translating problems, and developed intensely, covering from the development to control of complex physical phenomenon. It is essential to understand complex systems phenomena as a “*third method*” of research, construction and design, combines many advantages theoretical, numerical and experimental, Figure 3. The impressive progress in means of processing, transferring and storing information corresponds to the globally towards complication and overlap in various spheres of human activities.

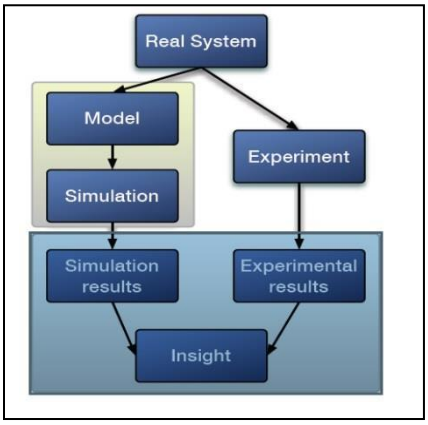


Fig. 3: Simulation gives the numerical solution to the model applied to a specific situation (Hans Fangohr, University of Southampton, UK)

Simply, a mathematical model is a set of mathematical statements:

$$M = \{\Sigma_1, \Sigma_2, \Sigma_n\}.$$

The above attempt of a definition is incomplete since it pertains to the word “mathematical” of “mathematical model” only, without any reference to purposes or goals. Following the philosophy of the teleological definitions of the terms model, simulation, and system, let us define instead

A mathematical model is a triplet (*S*, *Q*, *M*) where *S* is a system, *Q* is a question relating to *S*, and *M* is a set of mathematical statements $M = \{\Sigma_1, \Sigma_2, \Sigma_n\}$ which can be used to answer *Q*. Mathematical modeller with mathematical background with expertise techniques is important if one wants to solve more advanced system problems, but it is not necessary to be a professional mathematician if one wants to work with mathematical models.

Material scientific point of view, *M&M* is as a big resource of powerful methods and instruments to solve complex physical problems. Figure 4 visualizes this approach. A mathematical model (*S*, *Q*, *M*) opens up the way into the "mathematical universe", where the problem can be solved using powerful mathematical methods. This leads to a problem solution in mathematical terms (A*), which is then translated into an answer A to the original question Q in the last step.

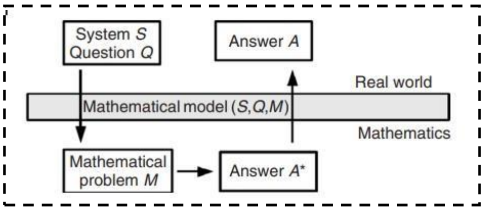


Fig. 4: Problem Solving Scheme

The "space of mathematical models" evolves naturally from Definition, where we have defined a mathematical model to be a triple (*S*, *Q*, *M*) consisting of a system S, a question Q, and a set of mathematical statements *M*. Based on this definition, it is natural to classify mathematical models in an *SQM* space. Figure 5 shows one possible approach to visualize this *SQM* space of mathematical models, based on a classification of mathematical models between black and white box models. Psychological and social systems constitute the "black box" end of the spectrum.

Note that the three dimensions of a mathematical model (*S*, *Q*, *M*) can be seen in the figure: the systems (*S*) are classified on top of the bar, immediately below the bar there is a list of objectives that mathematical models in each of the segments may have (which is *Q*), and at the bottom end there are corresponding mathematical structures (*M*) ranging from algebraic equations (*AEs*) to differential equations (*DE*s).

The "*Q"*-criteria in Figure 5a illustrate that mathematical models can be used to solve increasingly challenging problems as the model gradually turns from a black box to a white box model. At the black box end of the spectrum, models can be used to make more or less reliable predictions based on data.

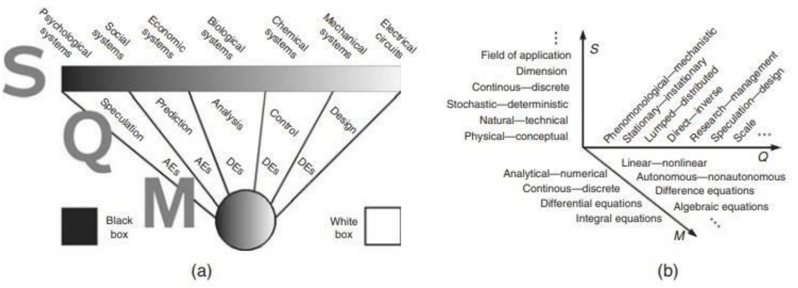


Fig. 5: (a) Classification of *M&M* between black and white box models. (b) Classification of *M&M* in the *SQM* space.

2.2 Principles of V-Model

Considering a classic "why-what-how" perspective for the development of a system, the "why" question is covered during the first stage (pre-concept), the "what" question regards the second stage (concept), and the "how" question is answered mainly during the subsequent two stages (development and production). It is also possible to analyse the system life cycle considering the core research, development and engineering (RD&E) activities developed at each stage.

The "pre-concept" and "concept" stages are focused in scientific development and the main activities relate with "discovery" (basic research, and research & engineering) and "innovation" (materiel solution analysis); during the "development" and "production" stages. The envolved processes, represented in the V-model, Figure 6.

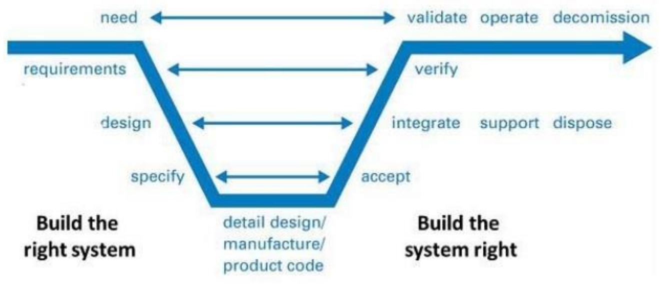


Fig. 6: System Engineering life cycle V-model

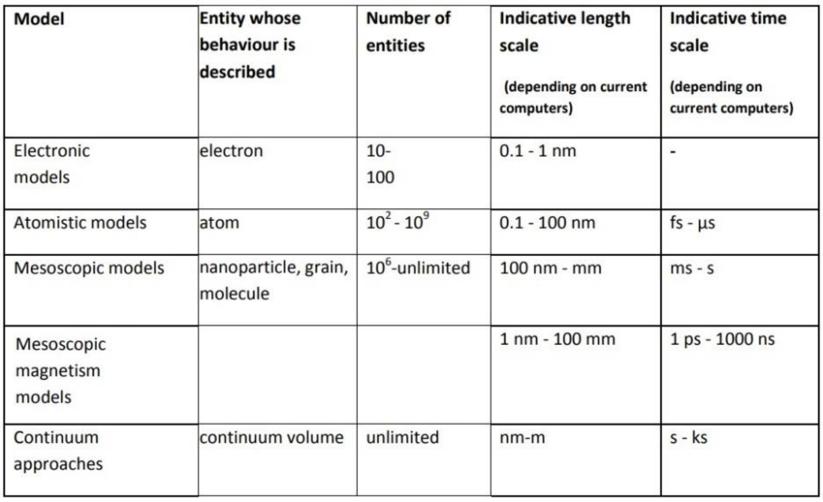
3. Concepts of Materials and Models

3.1 Model Development

Discovery and development of new and improved materials are at a rapid pace. Figure 7 from Professor Graham Schaffer‟s presentation to the advanced materials shows the considerations and factors that allow materials to perform in certain ways, known as the "*Materials Paradigm".*

The mathematical sciences, as a common language for the quantitative description of processes and phenomena, have their own unique role. Both the mathematical and materials sciences have much to gain from each other. The mathematical challenges in materials science vary with length scale, time scale, and temperature regime. The basic laws of these disciplines have very different mathematical structures and pose distinct challenges. Models are strictly classified according to the entity described by the physics and not according to the size of the application or system. The four natural categories of materials models consist of three discrete types and one continuum type of model, Table I:

Table I: Category of Material Models



Model	**Entity whose behaviour is described**	**Number of entities**	**Indicative length scale** (depending on current computers)	**Indicative time scale** (depending on current computers)
Electronic models	electron	10- 100	0.1 - 1 nm	-
Atomistic models	atom	10^2 - 10^9	0.1 - 100 nm	fs - µs
Mesoscopic models	nanoparticle, grain, molecule	10^6-unlimited	100 nm - mm	ms - s
Mesoscopic magnetism models			1 nm - 100 mm	1 ps - 1000 ns
Continuum approaches	continuum volume	unlimited	nm-m	s - ks

The use of materials models in industries is very versatile, which requires strong interaction between the code developers (software) and organisation/industry, and, because of the complexity and long timescale of the code development and validation process. The most crucial issue related to modelling process is in the formulation of models that produce realistic results. In general, *M&M* is as eyes of the experimentalists, to access information and interpret the experimental results. *M&M* provides also invaluable predictions on the evolution of a system in a quicker or cheaper way than with trial and error methods. *M&M* starts with an approximation which at first is seen as a good balance between complexity and computability. Development of models may either make the crude model more complex (and in principle the full physics equations will be retrieved again) or reduces the complexity of the model. Figure 8, is an illustration of model development, across time- and length-scales and Figure 9.

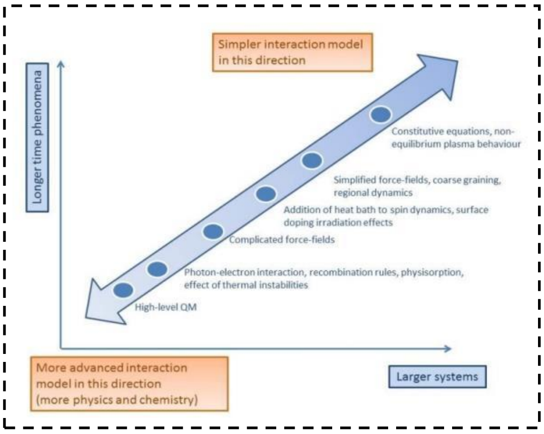


Fig. 8: Model development works by moving along the arrow upwards or downward

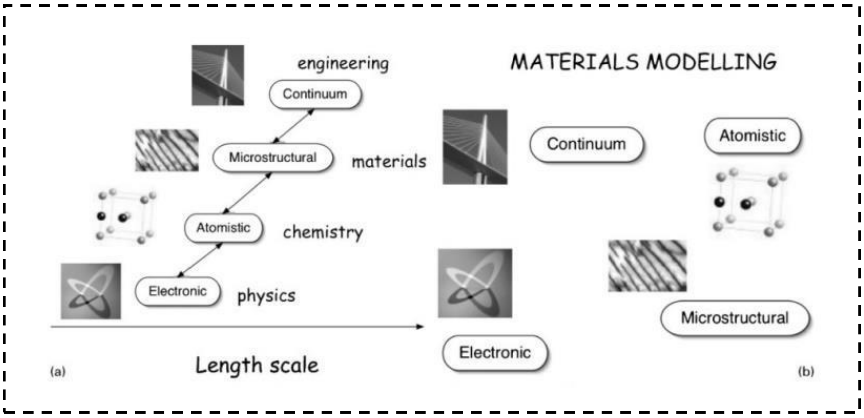


Fig. 9: Subjects vs Scales vs Disciplines

Materials are complex systems in nature. The equations that describe the physical and chemical behaviour of real systems are too complicated to be simulated or solved. In order to save (computer) time, the phenomenon has to be simplified in order to reproduce and predict experimental results. Key assumptions about reality are ignored due to the complexity.

Materials Models, an approximated *physics/chemistry equation* describing generic physics and its *closure relations* describing a specific material and its behaviour are called "*Material Model***".** In the materials domain the word "*materials relation*" is used for the closure relation, and it is note that "*constitutive equation*" is used in the continuum modelling world, Figure 10. Materials Modelling is the establishing of governing equations (physics/chemistry equations and/or closure relations) between physical or chemical quantities. These governing equations contain the key assumptions of the model. Modellers start from the strongly approximated physics equations, and gradually add complexity to it until a satisfactory agreement with experiments is reached.

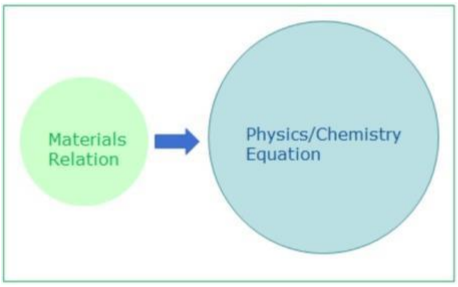


Fig. 10: Model with Governing Equations

Development of models may also reduce the complexity of an existing model with satisfactory accuracy. Modellers have also established new constitutive equations either from measurements. New constitutive equations linking physical or chemical parameters in a new empirical equation found as results of modelling or as results of experiments, are also included as new modelling. *M&M* are classified as follows: (i) those which lead to an unexpected outcome that can be verified (ii) those which are created or used in hindsight to explain diverse observations (iii) existing models which are adapted or grouped to design materials or processes (iv) models used to express data, reveal patterns, or for implementation in control algorithms. This "testing of models" is also a valuable part of modelling. The choice of a model depends on the balance between accuracy and simplicity. The outcomes of such testing might also be important because if none of the models are adequate the result of testing is that more physics/chemistry needs to be added to existing models.

3.2 Advantages of Material Models

- Saving costs by establishing a strategy for testing or it would be too complicated, dangerous or expensive.
- Understanding results of measurements.
- The simulation provides information for every point in the sample at every time.
- Reducing the time to market, by accelerating the time scales of understanding and developing new materials and new applications.
- Suggesting new materials and experimental procedures to create them. *M&M* can be used to examine the properties of materials and devices that have not or cannot yet be created.

4. Conclusions

MS is broadly concerned with the nature, properties, and use of materials. The *M&M* as a common language for the quantitative description of processes and phenomena has their own unique role. In particular, *MS* is today a vast and growing body of knowledge that is based on the physical sciences, engineering, and mathematics. Physics, chemistry, mechanics, and other traditional disciplines are now viewed as an arsenal of complementary scientific approaches serving the common goal of increased knowledge and understanding of all aspects of materials, from discovery and synthesis to products and uses.

Novel technologies and materials have resulted from these efforts. The biggest gains are when emphasis is on treating the problem at the level of complexity appropriate to technology. There is a need when comparing experimental data against models to be transparent on what is actually being validated.

Modern *M&M* can aid in solving significant problems in materials science, while problems in materials science can suggest fruitful areas for mathematical research. It is clear that the scientific vigour, technological strength, and economic health of the nation all support in favour of universities, government, industry, and professional societies stimulating and facilitating new collaborations between mathematical scientists and materials scientists.

References

[1] Principles of Mathematical Modelling – Clive L. Dym, Second Edition, 2004.

[2] Mathematical Modeling and Simulation Introduction for Scientists and Engineers - Kai Velten, Wiley-Vch Verlag, 2009.

[3] Principles of Modelling and Simulation: A Multidisciplinary Approach - J.A. Sokolowski and C.M. Banks (Eds.), John Wiley and Sons, Inc. New Jersey, 2009.

[4] Computational Approaches in Physics - Maria Fyta, Morgan & Claypool Publishers, 2016.

[5] What is Systems Engineering? Creating Successful Systems - H. Woodcock, INCOSE UK, 2009.

[6] **What makes a material function?** Let me compute the ways… Modelling in FP7 NMP Programme Materials projects, Fourth version, 2015, Edited by Anne F de Baas and Lula Rosso.

[7] Keynote to EDTAS Advanced Materials and Manufacturing Symposium- G. Schaffer, 2017.

[8] Modeling and Simulation in System Life Cycle - M.J. Simões-Marques, 6th International Conference on Applied Human Factors and Ergonomics (AHFE 2015) and the Affiliated Conferences, AHFE 2015, Procedia Manufacturing 3 (2015) 785 – 792.

[9] Cyber-Physical Systems: A Model-Based Approach - Walid M. Taha • Abd-Elhamid M. Taha Johan Thunberg, Springer, 2021.

[10] Continuous System Modeling – F.E. Cellier, Springer,1991.

[11] Aris, R.(1994). Mathematical Modeling Techniques . Dover, New York.

[12] Gershenfield, N. (1998). The Nature of Mathematical Modeling. Cambridge University Press, London.

[13] Upadhyay, R.K. (2013). Introduction to Mathematical Modelling and chaotic dynamics, CRC press

[14] Understanding Materials Science: History, Properties, Applications - Rolf E. Hummel, Springer-Verlag, 2004.

[15] Mathematical Research in Materials Science: Opportunities and Perspectives, 1993.