
Modeling

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Without doubt, “models and modeling” represents one of the most important core competences in industrial mathematics. Our primary purpose here is to clarify what we mean by models and modeling, for there are few terms in applied mathematics—perhaps few in all of the natural sciences—that have a wider variety of meanings and specialized uses. This is true, despite their also being key terms in natural science research, which is composed of the interplay between modeling and measuring.

So, let us begin with a definition of terms.

1 What Is a Model and what Is Modeling?

The literature is full of more or less original answers to this question. Here, for example, is an almost poetic entry: “Models describe our beliefs about how the world functions.” And, further: “With mathematical modeling, we translate the contents of our beliefs into the language of mathematics” [4].

One might also say that we form hypotheses and pictures of our beliefs about how the world functions—or at least a part of the world. There is a note of caution in such sentences. We don’t know how the world really functions, but we work with certain hypotheses about it until these hypotheses have been falsified. One hears the voice of Karl Popper here. These hypotheses have, at least, clear boundaries regarding the scope of their validity—and this is an important message, one that we place almost at the very beginning—especially when “world” means the world of industrial practice. Whatever is delivered in the form of solutions to industrial problems, one must never forget when applying these solutions that they were arrived at by virtue of simplified conditions that must

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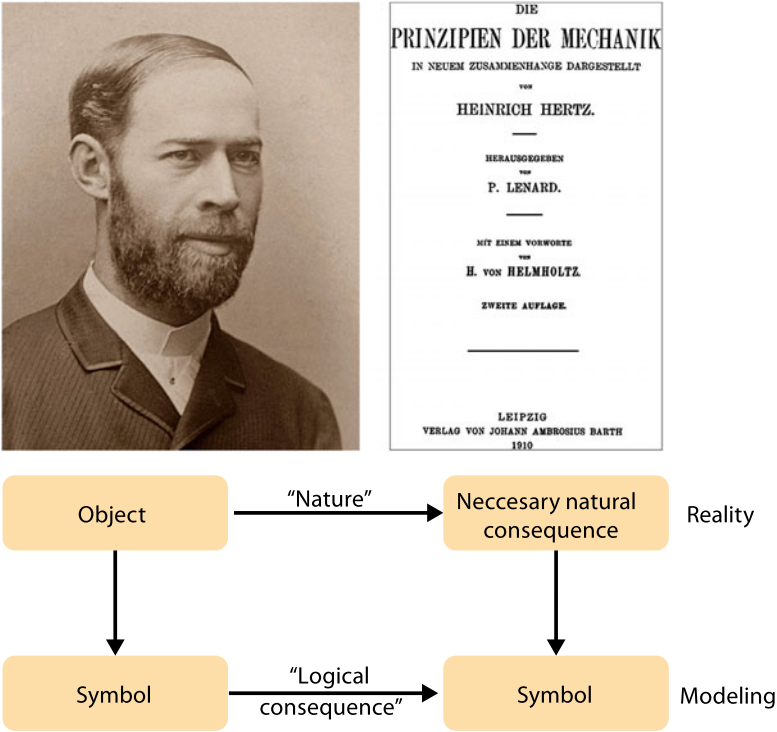


Fig. 1 Heinrich Hertz (1857–1894, Photo: Robert Krewaldt)

always be taken into account. This caveat has often been forgotten—in financial mathematics, for example—but also with regard to technical problems. The unreliability of the results was not the fault of the mathematicians, but of the blithe utilizers of the results.

However, it is also true that, within the boundaries of their validity, models can reflect the world with surprising accuracy—and this, above all, is what we want to discuss.

But let us remain for a while with the defining of terms. A less poetic definition than the first, but more useful from a scientific perspective, is that of the physicist Heinrich Hertz (Fig. 1), proposed in 1896 in his “Principles of Mechanics.” To quote Mr. Hertz:



Fig. 2 Systems: (a) natural ecosystem, (b) technical system (© Pressefoto BASF), (c) economic system (© Deutsche Börse)

“We create for ourselves internal replicas or symbols of external objects, and we create them in such a way that the logically necessary consequences of the pictures are always the pictures of the naturally necessary consequences of the replicated objects.”

In Fig. 1, we see a graphical representation of the above sentence. When we replace “internal replica or symbol” simply with model, then we understand that Hertz considered modeling to be the actual core of scientific research, for the above quote relates to the actual practice of science. We must determine the “logically necessary consequences of the pictures.” This works best when the pictures are “made up of mathematics.” Or, to put it another way: the raw material of the models under consideration here is mathematics. This corresponds to many other definitions of modeling also: “Mathematical modeling is the use of mathematics to describe phenomena from the real world” [7]. Moreover, the author goes on to say that modeling “investigates questions about the observable world, explains the phenomena, tests ideas, and makes predictions about the real world.”

Wikipedia puts it even more simply. Here, a model is the description of a system by means of mathematical concepts and language. A model can help to explain a system and study the influence of various components, as well as help to make predictions about its behavior. Here too, science and modeling are closely coupled: “The quality of a scientific field depends on how well the mathematical models developed on the theoretical side agree with results of repeatable experiments.”

A more thorough introduction to the most important terminology is provided by Velten [6]. He gives very formal definitions that are indeed correct, but not always helpful. The most comprehensible is still his Definition 1.2.1, which he adopts from Minski [3]: “To an observer B, an object A^* is a model of an object A to the extent the B can use A^* to answer questions that interest him about A.” Is it now clear to everyone what modeling means? Another basic interest of modeling and modelers is objects. In most texts—and in [6] as well—these objects are quickly made more specific: one is interested in systems: natural systems, such as lakes; technical systems, such as installations and motors; economic systems, such as the stock market; and virtual systems, such as computer games (Fig. 2).



Fig. 3 Model and reality: which is which? (© iStockphoto (*left*), Photo and montage: G. Ermel, Fraunhofer ITWM)

There are also more and less formal definitions for the term “system,” but we accept the word as it is commonly understood. Without exception, the work of the ITWM also deals with systems of the kind mentioned above: spinning installations, grinding equipment, filter systems, generators, stock markets, etc. And although we prefer Heinrich Hertz’s definition for our work and for this book, we too refrain from defining what a “picture” or replica is. We can say, however, that it illustrates to the investigator the essential qualities of a system; consequently, it excludes the non-essential qualities. In other words, a picture abstracts. Perhaps the word “caricature” would be more accurate than picture. Or perhaps the photograph in Fig. 3 says it best, entirely without words.

For us, then, a model is a picture of a system. The picture is composed of mathematics and reflects with satisfactory precision certain characteristics of the system that are of interest to the investigator. The model has clear boundaries for its validity, although these boundaries depend on the degree of precision that is desired. There are often parameters in the models that can be determined directly by measurement or extracted indirectly from measurement data via parameter identification. The precision requirements of the model must correspond to the precision of the data; it makes no sense to incorporate the tiniest phenomena into the model, when the parameters that belong to them can not be measured or can only be roughly ascertained—a problem that appears particularly often in biology. A cell’s metabolism is extremely complex. On the basis of the structure model shown in Fig. 4, a mathematical model can easily be constructed using a system of ordinary differential equations, but the many transfer coefficients are neither measurable nor identifiable.

Modeling is a significant part of scientific practice. Physics, for example, consists of modeling and measuring. Newton's mechanics, Einstein's relativity theory, and Schrödinger's quantum physics are just as much models as Navier–Stokes or Euler equations, as Darcy's law of flow in porous media, as Cosserat's solid body theory, or as the Maxwell equations. In our projects, classical physics predominates—particularly continuum mechanics, thermodynamics, and electrodynamics—since the temporal and spatial magnitudes dealt with in industry are generally well-suited to it.

The supply of models in biology or the social sciences is not nearly so plentiful as in physics, and one often has to invent them anew. This is a challenge and sometimes a joy as well, but here, one is not as firmly rooted in solid ground as in physics.

Ultimately, I believe that modeling, as we have outlined it here, is essential for all problem solving, and thus represents a fundamental human activity. For, as Karl Popper reflected: “Life is problem solving.”

2 Why Do We Model?

This question becomes superfluous once one has grasped what a model is. Nevertheless, the importance of mathematical models—and with it, the importance of mathematics—has increased greatly for industry, since computers have made it possible to utilize even more complex models. When one uses a computer to numerically evaluate a model that reflects a particular system, then one obtains in the computer a virtual picture of the system's behavior.

We simulate the system. A simulation thus arises by means of the numerical evaluation of models, generally with the help of a computer. A simulation allows the behavior of a system to be predicted; one can investigate how system changes impact behavior and one can also optimize systems using a computer. Thus, models and simulations serve as important supports for decision-making: tactical decisions in the case of managers, and strategic decisions in the case of planners.

In the days of Heinrich Hertz, most models could not be evaluated. One had to simplify them—for example, by reducing the number of dimensions from three to two, or even one, or by using perturbation methods—in order to be able to then “solve” the simplified models analytically. The solutions of such simplified models often help one to better understand the system: Which parameters are important? Are there bifurcations? Can the system become unstable? And so on. However, if one wants to quantitatively predict system behavior in real, three-dimensional systems—and technical systems are mostly three dimensional—then such simplifications are not acceptable, and one must try to find at least an approximate evaluation of the original, complex model (Fig. 5).

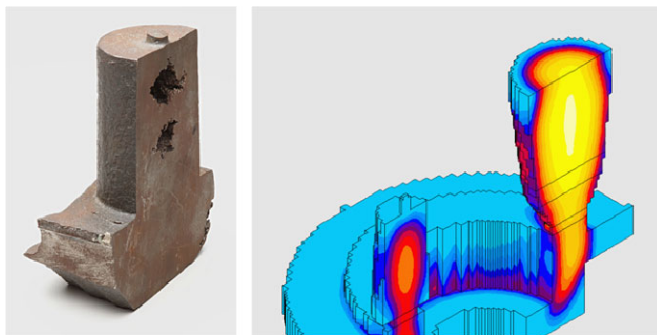


Fig. 5 Real and virtual systems: a cast object and a solidification simulation (Photo: G. Ermel, Fraunhofer ITWM; simulation: Fraunhofer ITWM)

In industrial practice, one almost always wants relatively exact quantitative predictions. A purely qualitative understanding is indeed useful, but usually insufficient. This question also distinguishes between various groups offering “industrial mathematics” as a university or research institute topic. The “Study groups with industry” founded in Oxford some 45 years ago, for example, bear down for an entire week on industrial problems using mathematical methods and deliver interesting analyses, but rarely quantitative predictions. The Fraunhofer ITWM, in contrast, strives to ultimately provide the client with software for simulating, optimizing, or controlling the systems. The two approaches also call for different working tactics. At the Fraunhofer, the models should be “as simple as possible,” but no simpler. A “small parameter” that is allowed to approach zero in Oxford in order to permit further investigations of the models is, at the Fraunhofer, often not small enough to cancel out without causing substantial quantitative errors.

Moreover, right from the start, when setting up the models, it is necessary to keep in mind that one must be able to efficiently evaluate them. Modeling and computation go hand in hand; artists of pure modeling and computation virtuosos, one without the other, are often inadequate to the real demands of industry. This calls for a genuine balancing act, for there are also “number crunchers” who will resort to faster algorithms, better computers, and sometimes coarser grids in their desire to evaluate the most complex of models—sometimes paying the price of large quantitative inaccuracies. Or of prohibitively expensive computing times. Modeling and computation specialists should form a team from the very beginning if they want to deliver reliable software to the client in the end. However, the idea of starting with the development of so-called “computer models,” that is, with models formulated directly in the language of finite elements (FEM), for example, is untenable in our opinion. Numerical methods, such as FEM, help with the evaluation of differential equations, which in turn represent models from continuum mechanics or electromagnetism. The models are one thing; their evaluation algorithms are another. There might indeed be, for example, more efficient algorithms than FEM, and one loses out on the chance of using them.

Nor does it make sense to set up models that cannot be evaluated. Such models were occasionally found in the past with system biology problems, where the systems of ordinary differential equations used for the modeling contained so many unknown parameters that no parameter identification algorithm could reliably calculate them all (see Fig. 4). Here as well, close cooperation between modeler and computation expert is needed to ensure that optimal use is made of the existing information.

So, to repeat the question: Why do we model? We model so that, in the end, we can simulate, optimize, and control a real system—within the virtual world of a computer. The picture from Heinrich Hertz comes to mind again. The simulation should replace real experiments, since it is simpler, faster, and cheaper. Imagine the geometry of a production line, of a car, of a chemical reactor; how much easier it is to vary them in a computer than it is in reality! But always with the caveat, the simulation must also be reliable.

Optimization algorithms can only be executed in the virtual world—the raw gemstone must be “virtualized” before it can be optimally cut or ground. Gerda de Vries [7] has one more argument: “Experimental scientists are very good at taking apart the real world and studying small components. Since the real world is nonlinear, fitting the components together is a much harder puzzle. Mathematical modeling allows us to do just that.”

Modeling and simulating is problem solving. We are always doing this, wherever we may find ourselves—though we are not always doing it consciously. However, this fact should be made conscious at an early age, while we are still in school. The models don’t have to be differential equations; counting and adding can suffice for model evaluation purposes. It represents great progress that modeling is included as a permanent topic in school instruction plans in some federal states of Germany. This book also includes a chapter that reports on the valuable experience with modeling that Kaiserslautern’s mathematicians have gained in schools (cf. “The training”). Just how deeply this look at modeling can penetrate into our daily life was made clear to me when taking leave of a Burmese student after her completion of a two-year Masters in “Industrial Mathematics.” “I cannot open a refrigerator any more without thinking about how I can model the cooling loss and change the controls so that the energy consumption is lowered,” she said laughing, and full of pride.

3 There Is Never Just One Model. How Can We Find the Right One?

Naturally, there is never just one model, not even when the questions about the system under consideration have been very clearly and unambiguously formulated.

For one thing, the model will depend very strongly on the modeler’s previous knowledge and experience. Perhaps the modeler only finds problems that are reconcilable with his existing knowledge base. I used to poke fun at how often my Oxford colleagues managed to discover “free boundary value problems, until I found myself discovering an astonishing number of problems that fit into the even more exotic area of kinetic equations. Of course, that should come as no surprise. “Very many, perhaps the majority, of people,

in order to find something, must first know that it's there," said G. Ch. Lichtenberg in his *Sudelbücher* book of aphorisms.

Naturally, only university mathematicians can afford such a luxury; when they search out their modeling problems, their search is "method driven." The mathematician at Bosch doesn't have this option. He has to optimize the transmission, regardless of what method fits. The Fraunhofer ITWM also takes on all problems that are mathematically interesting (and which lie within the Institute's competence). Granted, a problem may be transferred to the department that has the appropriate method for it. To be perfectly honest, however, departments usually attract the problems that suit them, which makes such problems transfers relatively rare.

Even when the modeler's methodological competence is not the determining factor, the model of choice is not unambiguous. Again, we see varying degrees of complexity. One begins with the "full physics" (models of first principles)—for example, the full compressible Navier Stokes equations—and, since these are not utilizable for the given parameters, ends with Prandtl boundary layer equations or with simpler turbulence models. This is the true art of industrial mathematics: how far can I drive the simplifications without violating my precision requirements for the simulation? Naturally, asymptotic analyses yield an error on the order of (ϵ^k) and a numerical error on the order of (h^p). My ϵ and h are small, but not zero, and these orders tell me absolutely nothing about the size of my error for a given ϵ and h . And the constants in the order estimations are much too rough to be usable.

One must validate the models and simulations in order to know what is really meant by "as simple as possible, as complex as necessary." We return to this point in the section "How do we construct the correct model?"

Here, however, we must still discuss the structure of the system somewhat. Actually, these are always input-output systems. They take input data, such as the environmental conditions or the tributaries to a lake, the control values of a machine, the trading data on a stock market, or the use of topography or solar irradiation in a solar farm, and convert it to output data, such as the lake's algae growth, the performance or consumption of the machine, the stock market quotation, or the daily energy production of the solar farm (see Fig. 6).

The system is the "piece in the middle" that transforms the input into the output. What this transformation looks like depends of course on the "state" of the system. Along with state variables that describe the system's instantaneous condition, there are also parameters that distinguish the system from other, similarly structured, systems. With an engine, for example, the geometry and fuel are described by parameters, while the temperature, pressure, piston position, etc. are state variables. The model's job is to describe their changes over time for a given input. The output is then usually a direct function of the state.

When there are natural laws that describe these state changes, such as the flow dynamic equations and the equations governing the combustion process in an engine, then all parameters have a geometric, physical, or chemical significance, and one can measure them. The model is then built from these equations, which often come from different areas of physics—one speaks then of "multi-physics"—and the measured parameters are



Fig. 6 Another example of an input-output system: a solar collector farm (© Siemens)

inserted. When the equations can be solved numerically with enough accuracy, then the input-output system can be simulated, and the output can be calculated and predicted for each input, without experimentation. Even better, one can change the parameters—say, the geometry or the materials—and then calculate how the output changes. In this fashion, one can try out ways to improve the output, for example, to reduce fuel consumption and harmful emissions in the engine and/or increase performance. And still better, one can optimize these criteria by varying the parameters; one can develop an “optimal engine.” Here, however, one should proceed cautiously. There are usually several criteria to be minimized or maximized; that is, one almost always has a “multi-criteria” problem. This will be discussed further in “The Concepts—Optimization Processes.”

There was a time when many companies used optimization algorithms to help them “calculate” the form of an auto body. This led to autos that all looked the same, once their decorative elements were stripped away. Today, one often foregoes the absolute optimum in favor of a little individuality.

Optimization algorithms require many evaluations of the target function(s), and each evaluation requires a simulation. Consequently, one must simulate the system many, many times, which means that the individual simulation runs cannot take too long. Model simplifications are called for here, at least for the initial optimization steps. The clever coupling of optimization and model/computation is an important, modern research area, about which we will likewise report elsewhere in this book (cf. “The Concepts—Optimization Processes” and “The Research—Maximum Material Yield for Gemstone Exploitation.”)



<http://www.springer.com/978-3-662-48257-5>

Currents in Industrial Mathematics

From Concepts to Research to Education

Neunzert, H.; Prätzel-Wolters, D. (Eds.)

2015, VIII, 437 p., Hardcover

ISBN: 978-3-662-48257-5