



Editorial

Grasping Complexity

The century of complexity has come. Many people write and speak about complexity. The statement of the great physicist Stephen Hawking, “I think the next century will be the century of complexity”, in his ‘millennium’ interview on January 23, 2000 (San Jose Mercury News) became a widely cited prophecy.

The face of science has changed (see cartoon in Fig. 1). Surprisingly, when we start asking about the essence of these changes and then critically analyze the answers, the result are mostly discouraging. Why do we talk about complexity? Somebody might answer that now we have to study *non-linear* systems and therefore they are complex. The answer seems to be plausible, nonlinearity results in non-additivity of parts and in the emergence of new phenomena: “The whole is more than the sum of its parts”. But objection appears immediately: non-linearity has been in the focus of scientific research already for more than a century. Poincaré and Lyapunov have studied nonlinear systems more than a century ago. Boltzmann’s equation and Navier–Stokes equation, the great nonlinear equations are more than a century old. Many ideas have been created and many methods developed. The study of non-linearity is not a symptom of the change of era. More than a thousand years ago Aristotle had written that “the whole is something besides the parts” (Metaphysics, Book 8, Chapter 6) and the Western culture had accepted this idea from the very beginning. By the way, ‘besides’ in this translation of Aristotle sounds much more precise than the widely spread ‘more’.



Fig. 1. Change of era: The direction is changed dramatically and the history of our motion is like a hood behind our shoulders. To describe our recent direction we need to understand our past. Graphics by Mikhail Molibog.

We need another idea to understand the recent change of era and some people add that we have to study large systems, both large and non-linear. Does the idea of *large dimension* give us the key for understanding of new era? Not precisely! The curse of dimensionality is now a well known problem and the term was proposed by Bellman in 1950s [1]. Fifty years before, in 1900, David Hilbert in his address to the International Congress of Mathematicians in Paris has described 23 major mathematical problems to be studied in the coming century [2]. The title of one of these problems sounds very strange and too broad “Mathematical treatment of the axioms of physics” but if we read beyond the title then we immediately realize what has been the main problem for Hilbert: “As to the axioms of the theory of probabilities, it seems to me desirable that their logical investigation should be accompanied by a rigorous and satisfactory development of the method of mean values in mathematical physics, and in particular in the kinetic theory of gases”. He continues: “Boltzmann’s work on the principles of mechanics suggests the problem of developing mathematically the limiting processes, there merely indicated,

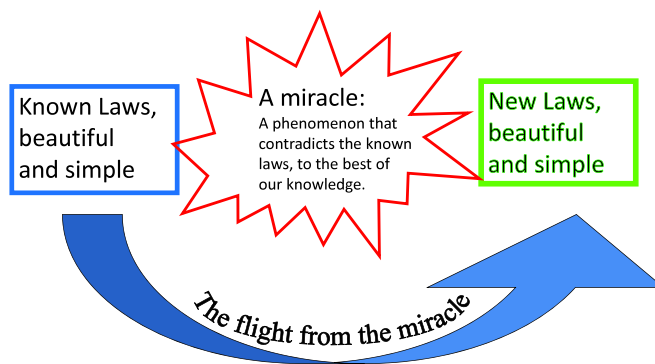


Fig. 2. The flight from miracle: Einstein's road.

which lead from the atomistic view to the laws of motion of continua". In the modern scientific jargon, Hilbert had asked about the correct methods of level jumping and model reduction, from large number of interacting particles to mechanics of continua. For this purpose, he proposed to develop the theory of probability and other related disciplines. This is the struggle with complexity of large nonlinear systems recognized as one of the most important problems for mathematics of the 20th century.

It is normal when the change of epochs under close examination looks as a continuous development, not as a jump. But we talk about a new century of complexity and suddenly find that it was started more than a century ago. Perhaps, the idea 'nonlinearity+large dimension' cannot separate the new era in spite of its attractiveness and clearness. To understand the essence of changes we have to ask not only what appears but also what has gone (Fig. 1).

What have been the most important scientific achievements of the 20th century? The new great laws: the great parade of the great discoveries, from the relativity and quantum mechanics to genetics and DNA. One of the main players of this great period, Albert Einstein, has described the discovery of the new laws as a "flight from miracle": "The development of this world of thought is in a certain sense a continuous flight from the 'miracle'." ["Die Entwicklung dieser Gedankenwelt ist in gewissem Sinn eine beständige Flucht aus dem 'Wunder', " [3].] What does it mean? Let us imagine: we have the laws, beautiful and simple (the Newton mechanics, for example). We find a phenomenon that we cannot describe using these laws. This is a *miracle*, a phenomenon that contradicts the basis laws. We trust in these laws, we know that they are supported by the previous development of science, we like them and try to use them again and again to describe the miracle. If we fail then we have to use another way. We like our laws but we like the rationality more, therefore we fly from the miracle by inventing new laws, which are beautiful, simple and, at the same time, allow us to describe the phenomenon. After that, the miracle disappears and we have new laws, beautiful and simple (Fig. 2).

This scheme can be explained much deeper with more historical details and examples, but the main steps are clear: we look for a miracle and find a phenomenon that seems to be in contradiction with the basic laws; we try to demystify this miracle by rational explanations and models based on these laws; after several attempts and failings we decide that new laws are needed and try to find new beautiful and simple laws that demystify the new phenomenon and still can explain the other known phenomena not worse than the old laws.

A new scheme of actions became dominant in the struggle with complexity. The complexity is recognized as the gap between the laws and the phenomena. We assume that the laws are true. We can imagine a 'detailed' model for a phenomenon but because of complexity, we cannot work with this detailed model. For example, we can write the Schrödinger equation for nuclei and electrons (formally, using indexes and signs of summation) but we cannot use them directly for modeling of materials or large molecules. We can imagine a detailed kinetic equation for a reaction network but cannot find reaction rate constants and cannot work with this large system even if it is true.

In some cases, bridging this gap between the laws and the phenomena can be achieved in model engineering by the special interaction between theoretical and experimental studies, and real engineering as well. Both the basic theory and the experiment will support the process of modelling. They may substitute for each other. For example, we can make experiments instead of solving the extremely complicated equations. We are sure that the answer should be the same after filtering the noise for experimental errors. We also can organise computational experiments instead of real ones. Again, we are sure that the answer should be the same after cleaning the results from the errors. In the background of this belief there is the fundamental assumption that the possible world of the theory coincides with the real world of our experiments and practice (with sufficient accuracy). We can believe that somewhere else, for high energies, very small distances, or very large distances we need new laws, but not now.

The interaction between theory and experiment in the model engineering may generate not only mathematical models but new experimental technics as well. For example, in chemistry, non-steady-state activity screening can be based on the technique of Temporal Analysis of Products (TAP), invented by John Gleaves in 1988. The main idea of TAP is to treat the catalyst by a series of pulses of very small intensity relative to the amount of catalyst [4]. This infinitesimal approach can be termed 'chemical calculus'.

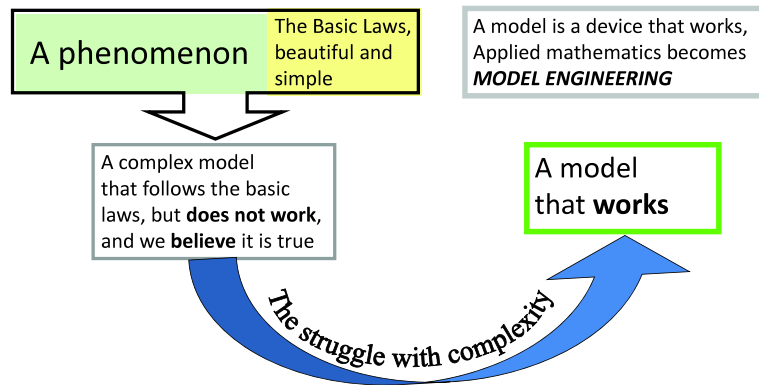


Fig. 3. Struggle with complexity: the life battle of the model engineers.

The result of the struggle with complexity is a model that works. This is a sort of engineering: a model is a device and this device should be functional. Applied mathematics and mathematical modelling become a sort of engineering and instead of Einstein's flight from miracle (Fig. 2) another scheme arises (Fig. 3): We know the laws and we have a phenomenon. We need a model for work. For different work need different models are needed. We may combine the first principles, the empirical data and even the active experiment to create the model. There exist special technologies for testing and validation of models. The structure of the whole process seems to be similar to the design of machines and it might be reasonable to teach the students in applied mathematics the module of 'Systems Engineering', as a guide the engineering of complex systems [5].

The focus has moved from the revolution in laws to the production of intellectual devices. In the context of the natural sciences this is model making under given basic laws. On the other hand, the systems under consideration may be artificial and instead of the basic laws we deal with the man-made plans, projects and scenarios. Such systems as the Internet, social institutions, large plants, financial system and many other systems are now in the focus of attention together with natural phenomena. The hybrid systems, that obey the natural laws but experience significant influence of human activity and man-made projects are of great interest too, like climate or biosphere.

The nature does not change and there will be many new laws to discover. The application of science always exists too. The era of complexity is in the change of the *focus* of the research activity. From the epoch of the great scientific revolutions we have moved to the epoch of the intellectual devices, from the revealing the God's or Nature plan to the intellectual engineering at various scales that is necessary to provide tools for prediction of the results of human activity. The new epoch may be ended some day but this is difficult to predict.

The milestones of development rarely coincide with the ends of calendar centuries. We believe that the 'century of scientific revolutions' is situated between two giants, from L. Boltzmann to R.P. Feynman. Surprisingly, their contribution in the era of complexity is also huge. We can just recall Boltzmann's entropy [6] and Feynman's inventions of nanotechnology [7] or quantum computers [8].

In the struggle with complexity there are many specific problems and tools. This issue presents several slices of this activity:

1. Measuring complexity: the curses and blessings of dimensionality;
2. Model reduction and invariant manifolds;
3. Fingerprinting, criteria, and interpretation of experiments;
4. Modelling of classes of complex systems.

In the first part, *Measuring complexity: the curses and blessings of dimensionality*, the general problems are approached. The first general problem is the *curse of dimensionality*. V. Pestov [9] demonstrates how the curse of dimensionality affects the nearest neighbor search and the widely used kNN classifiers. He demonstrates how the performance of the kNN classifier in very high dimensions can become unstable. Then, he develops a procedure for the reduction of the multidimensional statistical learning problems to a one-dimensional problem by a Borel isomorphism of the spaces with measure.

High dimensional problems are not always complex. From a certain point of view, they look much simpler: the central limit theorem in probability and the advanced results about *measure concentration* [10–12] demonstrate how convex sets in high dimension become 'almost spheres', and typical distribution functions look like Gaussians. This phenomenon (we call it the *blessing of dimensionality*) was recognised first in statistical physics by Maxwell and Gibbs [13]. For multiparticle systems (under some technical assumptions) the microcanonical ensemble with the given values of energy is equivalent to the canonical one which can be represented by the entropy maximum with the same average energy. The Maximum of Entropy (MaxEnt) approach naturally appears in the limit of high dimension.

In the middle of the 20th century, after C. Shannon's works [14] and E.T. Jaynes papers [15], the MaxEnt approach became very popular as a maximization of the subjective uncertainty measured by the Boltzmann–Gibbs–Shannon entropy. In 1960,

A. Rényi invented non-classical entropies [16]. Csizsár, Morimoto, Tsallis and many other researchers developed this idea further, and now we have the rich choice of the entropies for many problems. This rich choice leads to the ‘uncertainty of uncertainty problem’: which entropy to use for the uncertainty measurement? A.N. Gorban proposes to use all the entropies together [18]. This approach results in a set of conditionally “most random” distributions. Surprisingly, this set allows constructive description. This new ‘Maxallent’ (Maximizers of all Entropies) method is based on the understanding of entropy as a measure of uncertainty which increases in Markov processes [17].

In the work of M. Grmela [19], the Dynamical Maximum Entropy Principle is elaborated. It covers equilibrium and non-equilibrium thermodynamics and gives new approaches to some classical problems. In particular, the classical Chapman–Enskog expansion in the theory of Boltzmann’s equation [20] is described by the entropy deformation.

A. Zinovyev and E. Mirkes develop the data approximation approach to measure the complexity of datasets [21]. They utilize the universal approximators, principal cubic complexes that generalize the notion of principal manifolds and graphs [22] for datasets with nontrivial topologies and are constructed with a grammar of elementary graph transformations. Three natural types of data complexity are used and tested in the case studies: the geometric, structural and construction complexity.

Idempotent and tropical mathematics provide asymptotic versions of the classical mathematics produced by the ‘dequantization’ procedure [23]. G.L. Litvinov evaluates the complexity of the algorithms for the idempotent problems and their interval versions and demonstrated that they may be much simpler than in the classical mathematics [24].

Model reduction is one of the major procedures in the struggle with complexity and section *Model reduction and invariant manifolds* in the issue includes papers about reduction of dynamical models. M. Slemrod [25] revisits the sixth Hilbert problem and demonstrates that the solution has to be negative for compressible gas dynamics: the hydrodynamic limit does not lead to the classical compressible Euler or Navier–Stokes equations. This situation differs from the incompressible limit [26]. The key to this analysis is provided by the exactly solvable reduction models discovered by A.N. Gorban and I.V. Karlin [27,28].

Slow invariant manifolds are the main tools for model reduction in dissipative systems [29,30]. The fast manifold traditionally attracts less attention and plays an auxiliary role. It is used mostly for projection of a motion on an approximate invariant manifold. V. Bykov and V. Gol’dshstein [31] demonstrate how to start model reduction procedures from fast manifolds and develop a theory of Singularly Perturbed Vector Fields (SPVF) with the main emphasis on fast invariant manifolds. The slow manifold appears as a by-product of this approach. The new approach is illustrated by the examples from chemical kinetics.

The Lam and Goussis Computational Singular Perturbation (CSP) approach aims to find both fast and slow manifolds for a system of differential equations [32]. It was developed for application in chemical kinetics. In their paper [33], P.D. Kourdis, A.G. Palasantz, and D.A. Goussis develop the algorithmic realization of CSP and apply it to important biochemical systems with oscillations, the NF- κ B signaling system.

The problem of model reduction for systems with symmetries is analyzed by B. Sonday, A. Singer and I.G. Kevrekidis [34]. They use the Kuramoto–Sivashinsky equation with periodic boundary conditions and a stochastic simulation of nematic liquid crystals as examples, and apply the eigenvector-based techniques for model reduction. They also use a new technic, Vector Diffusion Maps [35], that combines, in a single formulation, the symmetry removal step and the dimensionality reduction step.

B.R. Noack, R.K. Niven [36] develop further a MaxEnt closure strategy for Galerkin systems arising from a projection of the incompressible Navier–Stokes equation onto orthonormal expansion modes. They aim to discover and demonstrate a new face of the turbulence closure problem.

R. Hannemann-Tamás, A. Gábor, G. Szederkényi, and K.M. Hangos formulate the model reduction problem for chemical kinetics as a quadratic programming problem [37]. The objective function is derived from the parametric sensitivity matrix. The method eliminates unnecessary reactions for a given level of tolerance and adjusts the rate constants of the remaining reactions for error minimization. The efficiency of the approach is demonstrated on the known benchmarks.

The transition from dynamics to thermodynamics is the most complicated step on the stair of reduction [30]. In the paper by T. Chumley, S. Cook, and R. Feres [38] this step is analyzed for billiard-like random systems. These systems exhibit irreversible thermodynamics behavior, indeed.

The ideal model reduction technology starts from the detailed system and produces the reduced one. This picture may be oversimplified. Indeed, in many practically important cases the mathematical model cannot be produced without simplifications and model reduction becomes a tool for model construction from scratch. It may be also used for construction of semi-empirical methods and active theory-driven experiments. In engineering, many semi-empirical criteria were invented to separate regimes: laminar from turbulent, shocks from smooth incompressible flows and many others. The modern fingerprinting idea may find its logical roots in the semi-empirical criteria. “The goal of the fingerprint analysis is to find features and characteristics of observed complex behavior, based on which it is possible to find out the model, its class or its family, and to determine its characteristics” [39]. The fingerprints, patterns, signatures or motifs allow us to work with complex systems without extraction of deep and expensive information. Kinetic signatures in biochemical reactions [40], motifs of genetic sequences [41] patterns in time series [42] (cardiograms and encephalograms, for example) give us nice examples of fingerprinting.

The paper by D. Constales, G.S. Yablonsky, and G.B. Marin [43] opens Section *Fingerprinting, criteria, and interpretation of experiments*. They study the basic patterns in simple reaction networks. This work aims to analyze appearance of some basic

patterns in chemical kinetics, to review and extend the previous findings [44]. Authors supplement the classical notion of complexity by 'simplicity' to reflect the rich diversity of patterns which can be produced even by simple systems.

A useful example of a criterion validation is given in the work by F. Xia and R.L. Axelbaum [45]. They propose to use the local ratio C/O to classify various regimes and zones of diffusion flames. Radical pool and soot precursor zones are shown to be clearly delineated in C/O ratio space. This ratio is validated as a criterion for interpreting flame structure.

M.J. Hankins, T. Nagy, and I.Z. Kiss [46] develop an original technology for active experiment for construction of nullcline-based models and demonstrates its efficiency on the modelling of the electrochemical reaction. Perhaps, the first author who proposed to use the nullcline-based models instead of detailed differential equations was A.N. Kolmogorov [47,48]. M.J. Hankins et al. use the nullcline-based models with the singular perturbation assumption (time scale separation). Under this assumption, the nullclines may be extracted from the control experiment with a combination of active and proportional controllers acting on the fast and the slow variables.

The section *Modelling of classes of complex systems* includes four papers about four classes of systems: networks, finance, catalysis (in chemical engineering) and bioreactors. The new tools and case studies are presented. H. Sayama, I. Pestov, J. Schmidt, B.J. Bush, C. Wong, J. Yamanoi, and T. Gross describe the methods based on adaptive networks with self-organization of structure for modeling of complex networks like social, transportation, neural and biological networks [49]. B.E. Baaquie describes a quantum mathematics approach to financial modelling [50]. F.J. Keil presents a thorough review about modelling in catalysis, from quantum chemical methods for calculating reactions on the active centers to transport in porous media [51]. I. Iliuta and F. Larachi study dynamics of bacterial cells in trickle-bed bioreactors. They model the basic processes, fluxes in multiface flows, population balance for cells and agglomerates, biomass dynamics, dynamics of agglomeration and filtration [52].

Neither one issue of a journal, nor a large encyclopedia can capture everything about such a broad and dynamic subject as grasping complexity, but we hope that various faces of the modern era of complexity are presented here.

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