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Lectures of the Blaise Pascal Awardees

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Professor **Frans de Schryver, Leuven, Blaise Pascal Medal in Chemistry**

In recognition of his outstanding contribution to the study of photochemical polymerization, of dynamic processes inducing either photophysical or photochemical pathways. He studied systems involving polymers but also crystals at the liquid-solid interface and developed techniques to detect single molecules.

Frans Carl DE SCHRYVER
Department of Chemistry
University of KULeuven
Belgium

Frans De Schryver obtained the degree of doctor in sciences in 1964 and is since October 2004 professor emeritus of the KULeuven. He has been for many years involved in the area of photochemistry and photophysics. His research has focussed on fundamental aspects of photochemistry and photophysics and their use in the study of physicochemical properties of complex systems. During the last 10 years he contributed primarily to the emerging field of time and space resolved (photo)chemistry including scanning probe microscopy, optical microscopy and single molecule spectroscopy and nanoscience. He has published over 650 papers in peer reviewed journals. He is a member of the Belgian Royal Academy, EAS, Fellow of the Royal Society of Chemistry and Editor in chief of Photchemical and Photobiological Sciences, associated editor of ChemPhysChem and member of the Editorial Board of Angewandte Chemie and Chem Phys Lett. He has received a senior Humboldt research Award and a Max Planck research Award as well as the Forster, Porter and Havinga medals. His lecture, “Dancing with Molecules”, focuses on his present interest in single molecule spectroscopy

One of the most intriguing new aspects of physical chemistry is the possibility to address and visualize single molecules. As when dancing with a partner this can be done by eye contact (visual observation using fluorescence microscopy) or by touching (scanning probe microscopy). The research group has over the last decade been actively involved in both approaches.

In the lecture the advantage of single molecule detection will underlined and the basic methodologies will be briefly discussed and the principle of scanning tunneling microcopy will illustrated by a few examples.

Seeing : Optical detection.

Using confocal (figure 1) or wide field (figure 2) fluorescence microscopy it is possible to study the properties of a single molecule or single molecule event. This allows us to get rid of the ensemble averaging always present studying a large number of molecules in solution and permits to get a much deeper insight in the activity of the single event. It is however essential that also the excited state properties of the chromophores used in the study are well understood.

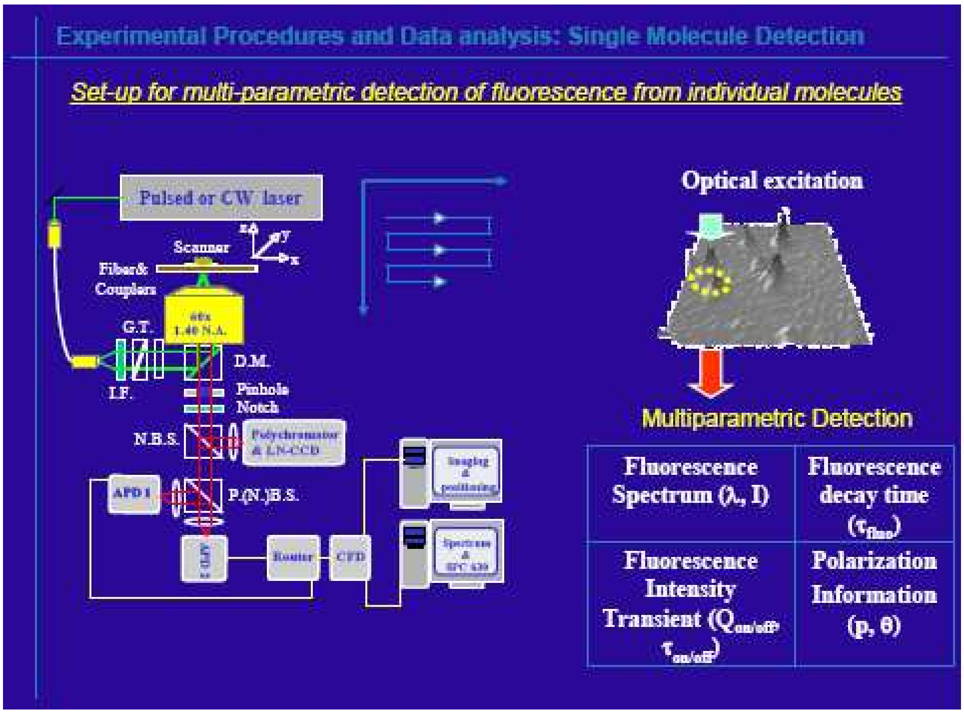

Figure 1 Single molecule detection by confocal microscopy

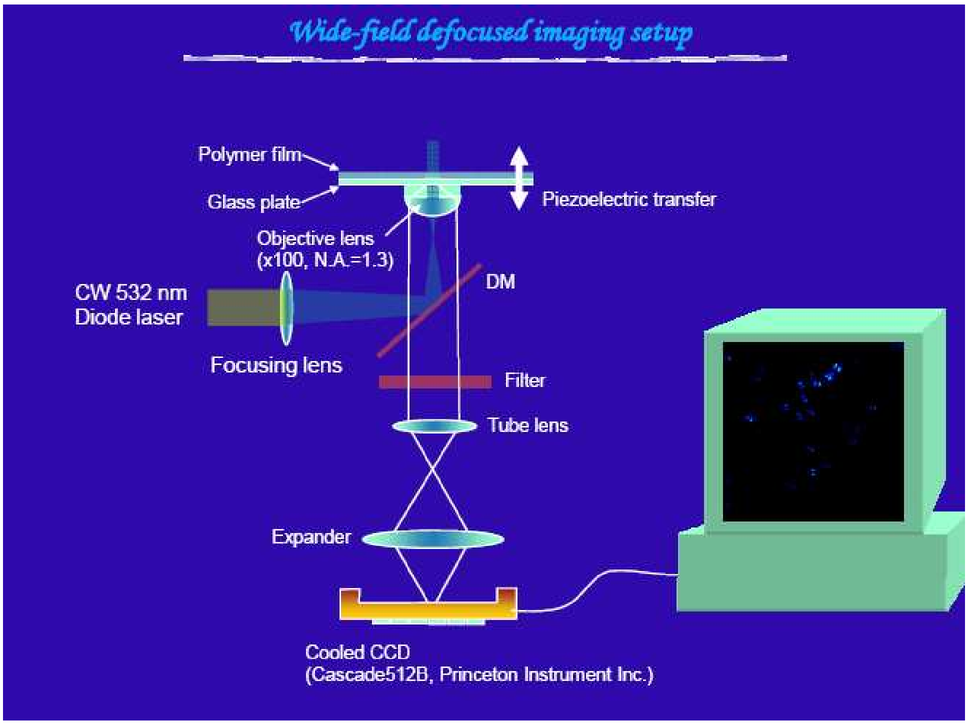

Figure 2 Wide field single molecule fluorescence microscopy

Therefore, fundamental photophysical processes are investigated as well at the ensemble, using femtosecond transient spectroscopy and tile correlated single,photon counting, as well as at the single molecule level. The combination of both approaches allows investigating in more detail especially those processes that can be considered rare events which usually are not or to a lesser extent observed in the ensemble spectroscopy. [1] The understanding of basic photophysics at the single molecule level opens novel possibilities to investigate complex systems (figure 3). It will be furthermore demonstrated that space resolved luminescence spectroscopy allows deeper insight in fundamental aspects of polymer physics [2] and catalysis [3] (figure 4).

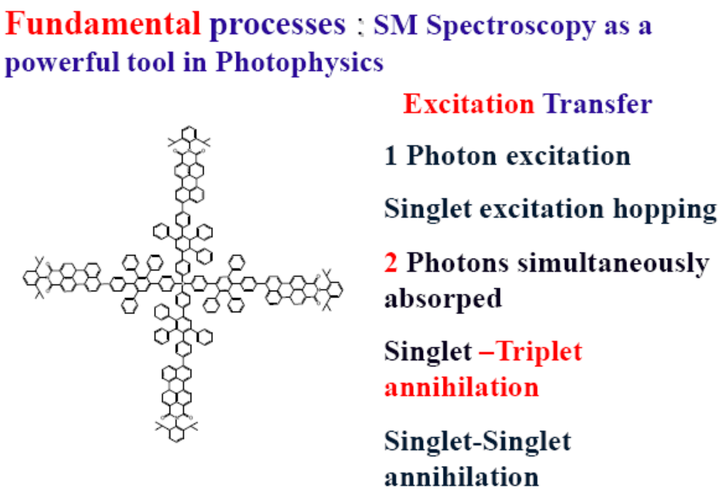

Figure 3 Fundamental processes in multichromophoric single molecules.
(Accounts of Chemical Research, 514-522 (2005))

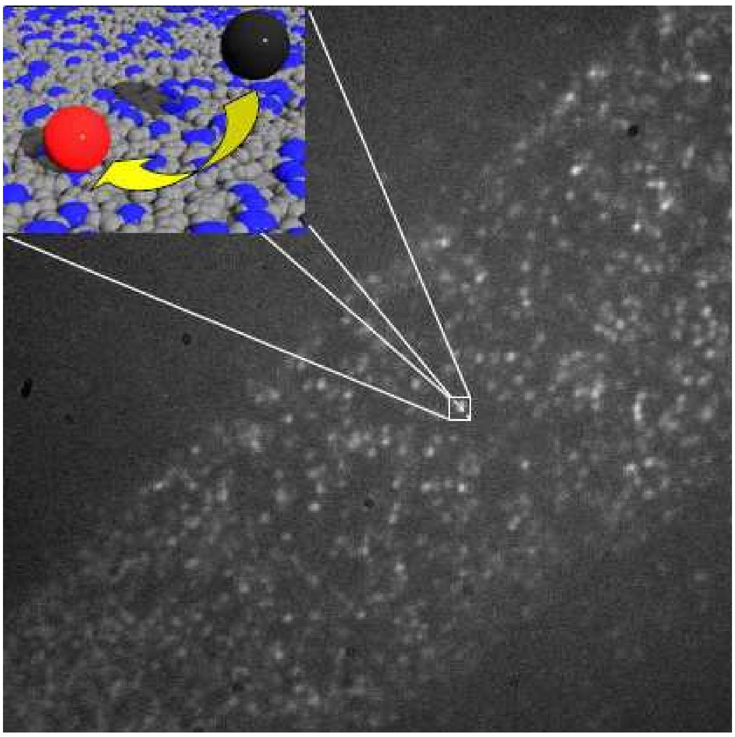

Figure 4 Visualization of a single catalytic event (PNAS 104, 12603–12609 (2007)).

Feeling: Scanning tunneling microscopy

Scanning tunnelling microscopy at room temperature allows investigation of single molecules embedded in a supramolecular structure with submolecular resolution.

- Local probe : sharp metallic tip. - Tunneling current between tip/substrate measured.
- Tunneling current modulated by molecule in gap. - Conducting, atomic flat surface needed.
- Atomic resolution can be achieved.

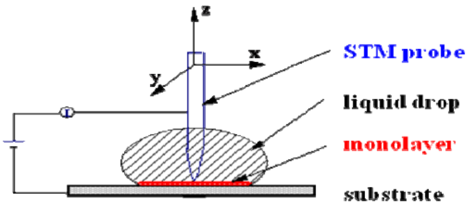

Figure 5 Principle of room temperature STM

When organic molecules dissolved in e.g. phenylalkane are adsorbed at a surface of HOPG as a monolayer one can image the structure by the variation in the tunnelling current through the molecules (figure 5) STM provides detailed insight into the importance of molecule-substrate (epitaxy) and molecule-molecule interactions (hydrogen bonding, metal complexation, fluorophobic/fluorophilic interactions) to direct the ordering of both achiral and chiral molecules on the atomically flat surface (figure 6). By controlling the location and orientation of functional groups, chemical reactions can be induced at the liquid/solid interface, via external stimuli, such as light, or by controlled manipulation with the STM-tip. The electronic properties of the self-assembled physisorbed molecules can be probed by taking advantage of the operation principle of STM, revealing spatially resolved intramolecular differences within these physisorbed molecules. [4]

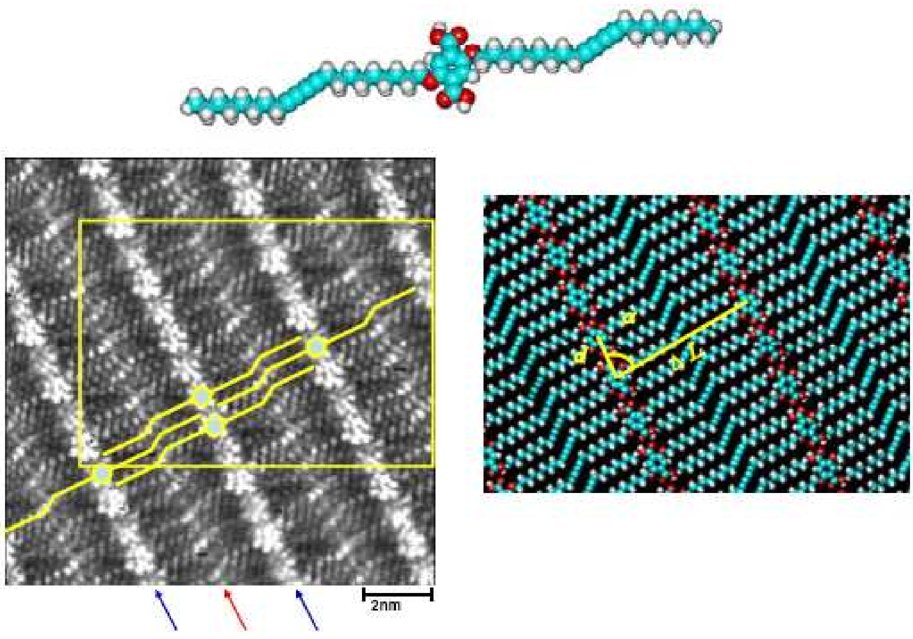

Figure 6 Molecularly adlayer imaged with submolecular resolution by STM and its model (blue arrows indicate the phenyl group and red arrows indicate the acetylenic group).

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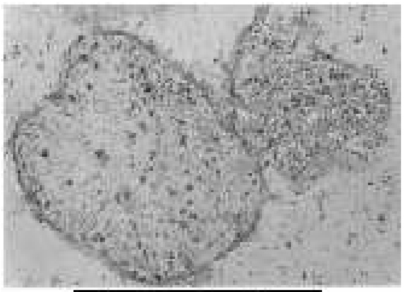
Professor **Howard Green, Boston, Blaise Pascal Medal in Biology and Life Sciences**

In recognition of his outstanding work on the development of cultivation of human epidermal cells to generate large scale autologous skin transplant. He discovered and developed to perfection his method to restore the skin of 3rd degree burn victims who were too severely burnt for conventional skin grafting. In the last 20 years this method has saved the lives of tens of thousands of burn victims all over the world.

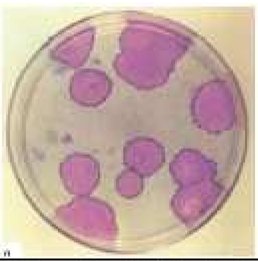
Howard Green
George Higginson Professor of Cell Biology
Department of Cell Biology
Harvard Medical School
USA

The Birth of Therapy with Cultured Cells

In 1974, I had no intention of studying therapy with cultured cells or the treatment of human burns. I was studying a serially transplantable teratoma or germ cell tumor of the mouse for totally different purposes. In the course of these studies, my graduate student James Rheinwald and I noticed that when the cells were cultivated, some of them gave rise to interesting colonies of epithelial appearance. We attempted to obtain the cells of these colonies in a pure state, but we were unsuccessful because the isolated cells would not grow. In order to support their growth, we added lethally irradiated cells of the line 3T3 that had been made in my laboratory years earlier. Under these conditions the epithelial cells grew quite nicely (Figure). But what kind of cells were they? When sections through colonies were examined by electron microscopy, they showed the presence of desmosomes, keratohyalin granules and aggregated tonofilaments. These are features of the keratinocyte, the cell type of stratified squamous epithelia, such as the epidermis.



Unstained colonies



Colonies stained with rhodamine

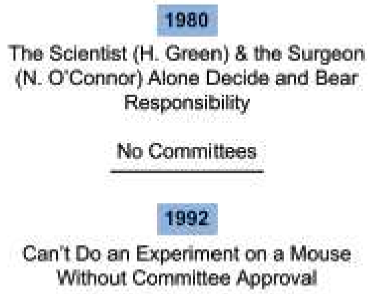
I knew that the human keratinocyte had never been grown to an appreciable extent in cell culture. So we obtained a fragment of human skin, dissociated the cells and put them into culture in the same way, with 3T3 support. They grew extremely well, each inoculated cell giving rise to a colony (Figure). Successive improvements in the cultivation made the keratinocyte the most proliferative of all cultured human cell types.

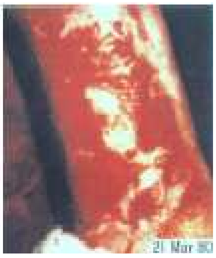
We then developed a method of making a graft out of the cultured keratinocytes and showed that such a graft, when placed on a wound in a mouse lacking immune resistance, would generate a human epidermis.

Having learned that we could grow vast amounts of such cultures and that they could engraft successfully on a mouse, we had to ask: could such a culture prepared from a human whose epidermis had been completely destroyed by a burn be used to regenerate his epidermis?

How the decision was made to attempt this experiment is shown in the figure. Notice that, in 1980, the two participants bore all responsibility. Notice also that by 1992, I was unable to do any experiment on a mouse without approval by a committee.

This kind of progress is called Regulation. It might also be called Strangulation.





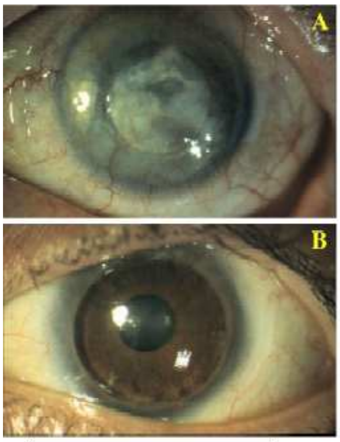
The first therapy of a human with a third degree burn with cultures made from a small fragment of his own skin was carried out in 1980. You can see the patches of regenerated skin on his arm resulting from circular cultures (Figure). Successive applications of such cultures resulted in complete coverage of the arm.

The next stage of development was to show that large-scale use of the method could be life saving. Two young brothers who were burned over more than 90% of their body surface and could not possibly survive with conventional treatment were treated with cultures prepared from their own skin (Figure). You can see here the application of now rectangular

cultures to the surface of the abdomen of one of the brothers and the complete regeneration of the skin 14 weeks later. Both brothers survived and lived for over 20 years before they died of complications not directly related to their burns.

When scientific discovery opens up a new field of research it is impossible to anticipate where it may lead. I now wish to turn to some unanticipated consequences of the discoveries that I have just described. Chemical burns of the eye, if they destroy the stem cells of the corneal epithelium, can lead to a very nasty condition of inflammation, pain and loss of vision. These stem cells belong to the same family as epidermal keratinocytes and they can be cultivated in the same way. A graft of such a culture to the eye will result in regeneration of the corneal epithelium.

This was discovered in the laboratory of Professors Michele de Luca and Graziella Pellegrini, right here in the European Union, more precisely in Italy, formerly in Venice and now in Modena. They took a 1-2 mm biopsy from the stem cell region of the healthy eye, grew the cells in culture, prepared a graft and applied it to the suitably prepared injured eye.



Before Treatment

5 years after graft of limbal culture
(4 years after corneal transplant to remove stromal scarring)

Rama, … and de Luca, 2001

In over 100 patients so treated, Professor de Luca’s laboratory, in collaboration with numerous ophthalmologists, obtained relief of symptoms in 80% of cases. With subsequent repair of deeper injury, vision could be totally restored (Figure).

Another unanticipated consequence of my work was the use of cultured keratinocytes for gene therapy. This was also developed in Professor de Luca’s group. They showed that a certain genetic disease producing severe blistering of the skin could be treated by culturing the epidermal cells of the patient, introducing a normal copy of the affected gene, preparing grafts from those cells, removing the affected skin of the patient and applying those grafts to the surface. The result was production of a normal epidermis and cure of the disease.

Conclusion

I have described how my work that gave birth to therapy with cultured cells was unplanned and was guided by the new possibilities that developed at each stage of the work. The unanticipated therapeutic applications of cultured keratinocytes were developed in the laboratory of Professors de Luca and Pellegrini. Many investigators throughout the world are now attempting to use cultured cells for therapeutic purposes, some more realistically than others. One group I would specially like to mention is that of Anders Lindahl and his collaborators in Gothenburg who developed a therapeutic use for cultured cartilage cells.

Professor **Alexander N. Guz, Kiev, Blaise Pascal Medal in Materials Sciences**

In recognition of his outstanding achievements in fundamental aspects of modern mechanics. He personally developed the theory of composite materials including all levels of composite material structure: macro, meso, and micro. He is also one well-known leader in the three-dimensional linearized theory of stability of solids.

Alexander N. Guz
Institute of Mechanics
Kiev, Ukraine

A.N.Guz graduated from the Mechanics and Mathematics Department of Kiev State University in 1961. He received the Doctor of Sciences degree (1965) and was was named Professor (1969). He has worked at the Institute of Mechanics of the NASU (National Academy of Sciences of Ukraine) since 1960, receiving an appointment as Head of the Department of Dynamics and Stability of Continuum Media (1967) and serving as Director of the Institute of Mechanics of the NASU (from 1976 until present). He is Academician of the NASU (1978), Member of the Academia Europaea (1992), Fellow of the New York Academy of Sciences (1997), Fellow of the World Innovation Foundation (2001), Member of the European Academy of Sciences (2002). His principal scientific results have been obtained in mechanics of deformable solids and related problems of continuum mechanics: the three-dimensional theory of stability of deformable bodies, the theory of propagation and diffraction of elastic waves in multi-connected bodies and bodies with initial stresses, stress concentration around holes in shells, mechanics of composites materials and structural members utilizing them, aerohydroelasticity, non-classical problems of fracture mechanics, rock mechanics, dynamics of viscous compressible liquid, contact problems, mechanics of nanocomposites and non-destructive methods of stress determination. He is the author or co-author of 55 books and about 900 scientific papers . He was awarded the Blaise Pascal Medal of the European Academy of Sciences (2007), the State Prize of USSR (1985), the State Prizes of Ukraine (1979, 1988), the Prize of the National Academy of Sciences of Ukraine (1979, 1983, 2000). He serves in the editorial boards of several international scientific journals and is the editor-in-chief of the international scientific journal Prikladnaya Mekhanika. He is the Chairman of the National Committee of Ukraine on Theoretical and Applied Mechanics .

Mrs. President, Colleagues, Ladies and Gentlemen:

I am regretting that I am not together with you at this **Ceremony of Awards** of the **Blaise Pascal Medals 2007**. It is very high honour to me to be awarded the **2007 Blaise Pascal Medal** in Material Sciences from the **European Academy of Sciences**. This high Award relates to my studies in fundamental aspects of modern mechanics as applied to Material Sciences. In view of its I would like to say a some words as applied to mechanics today in general.

First of all the specifity and place of mechanics in the existing modern system of scientific investigations must be taken into account. It can be assumed that mechanics specificity as the science consists in that mechanics is one of the major sciences of a fundamental character, and at the same time mechanics actuality is defined by the importance for engineering of studied nowadays problems. At all stages of the human progress, beginning from ancient times, the importance of mechanics for engineering can scarcely be exaggerated: in many cases, mechanics and engineering have been considered as a single whole.

Mechanics is transformed to present time into the very ramified area of knowledge. Some idea about diversity of problems considered in mechanics can be received from the written below information on separate scientific directions.

By the form of physical models used in phenomena studies, mechanics is divided on *rigid body mechanics, fluid, gas, and plasma mechanics,* and *solid mechanics*. If two or three of mentioned above models are used together for exploring the sufficiently complicated phenomena, then these investigations are referred conditionally to *general mechanics* or to the its separate directions such as, for example, *aerohydroelasticity*.

By the applied methods used in studies of phenomena, mechanics is divided on *analytical mechanics, computational mechanics,* and *experimental mechanics*. And besides, even international congresses are often organized separately according to mentioned above directions of mechanics. Let us note that general problems, including the formulations of a closed statement of problems, uniqueness theorems, variational principles and other related problems, are referred to analytical mechanics. At present time, analytical mechanics is treated in the broader sense, when corresponding problems of fluid, gas, and plasma mechanics are referred to the analytical one. Of course, methods and approaches corresponding to two or three mentioned above directions are applied together for a number of problem studying.

Sufficiently often, mechanics is divided on the separate scientific directions corresponding to the separate specific *directions of practical human activity*. When this approach is realized, then one can say, for example, about *space flight mechanics, civil-engineering or structural mechanics, composite materials mechanics, rock mechanics, structural mechanics of planes or ships, biomechanics, mechanics of a man, celestial mechanics,* and a number of other directions.

Solid mechanics is divided on *theory of elasticity, theory of plasticity, theory of viscoelasticity, creep theory, and fatigue theory* by the form of mechanical models used in the phenomena studied. Within the framework of this approach, one is also expediently to distinguish *mechanics of coupled fields in materials and structure members*, which studies the behaviour of materials and members of structural under the combined action of force, temperature, and electromagnetic fields.

Solid mechanics can be also divided on *statics, dynamics, stability,* and *fracture* by the character of mechanical phenomena considered. And besides, fracture mechanics investigates the mentioned phenomenon both under static and under dynamic loads. It is need emphasize that in the general case the fracture phenomenon has more complicate character and includes mechanical, physical, and chemical aspects. Therefore, the fracture phenomenon is investigated in the general case with taking into account mentioned above aspects.

Above, a series of directions in mechanics are shown as examples of a classification. At present time, the detailed classifiers of scientific directions in mechanics are elaborated in a number of states and specialized editions on mechanics. References on these classifiers are widely used in scientific results publications.

It is necessary to note that the next scientific directions in mechanics: *computational mechanics, mechanics of a space flight, biomechanics, mechanics of composite materials,* *fracture mechanics*, *mechanics of coupled fields in materials and structure members*, and also a number of other directions were actively developed in the second half of the XXth century.

My studies in modern problems of mechanics as applied to Material Sciences refer *to fracture mechanics*. In view of its I would like to say a some words on fracture mechanics today.

Fracture mechanics was one of the most actively developed fundamental and applied areas in mechanics in the latter half of the 20th century. Presently, this area in its topicality, fundamentality, and applicability to engineering may be compared only with the mechanics of composites. This is supported by the fact that two eight-volume collective encyclopedic monographs devoted to the two above-mentioned scientific areas were published in the midsecond half of our century.

Nowadays, we may apparently consider that fracture mechanics (in a broad sense) includes well-defined basic concepts and approaches to the formulation of fracture criteria. *The issues below may be classed as the basic concepts and approaches in fracture mechanics (in a broad sense).*

1. The fundamental Griffith theory of brittle fracture.
2. The concept of quasi-brittle fracture (Irwin, Orowan, and others).
3. The Griffith energy fracture criterion or the equivalent (more easily implemented) Irwin energy criterion.
4. The concept of an integral (J -integral, Γ -integral, Eshelby, Cherepanov, Rice) independent of the path of integration.
5. The critical crack opening criterion.

The above-stated concepts and approaches assume that *the following conditions* are satisfied.

Condition 1. Tension or shear arises near cracks, compression being excluded.
Condition 2. During the deformation, a cracked body does not change sharply its configuration (for example, buckling does not precede fracture).
Condition 3. During the deformation of a cracked body, the prefracture deformation pattern is not changed sharply (for example, subcritical crack growth and changes in the boundary conditions during deformation are absent).
It should be noted that Condition 1 is *principal one*, since the above concepts and approaches do not work upon compression along cracks.
Under Condition 2, all the above-mentioned concepts and approaches may work; however, a preliminary study should be made of the stress-strain state of a body sharply changing its configuration during deformation. Presently, such an analysis has not been performed in the overwhelming majority of studies in fracture mechanics (in a broad sense).
Under Condition 3, all the concepts and approaches may work; however, a preliminary study should be made of the stress-strain state of the body when the prefracture deformation pattern is sharply changed (for example, when the boundary conditions change during the deformation). Presently, such an analysis has not been performed in the overwhelming majority of studies in fracture mechanics.

Based on the foregoing considerations, results and problems corresponding to the above five concepts or approaches and obtained under Conditions 1-3 may be considered as the ***classical problems of fracture mechanics***, among which are the following studies.

1. Determination of the stress intensity factors for complex cracked bodies under various mechanical, thermal, and electromagnetic actions. To this end, analytical, numerical (computer-aided), experimental, and experimental-theoretical methods are applied. The results of these studies (stress intensity factors) together with the fracture criteria mentioned provide the necessary information on the fracture of materials and structural elements in cases where these fracture criteria are applicable.
2. Experimental investigation of the complex fracture of materials and structural elements. The results are mostly descriptive and obtained without due analysis and attempts to formulate new fracture criteria corresponding to the phenomena under consideration.
It is worthy to be noted that currently the overwhelming majority of publications pertains to classical fracture mechanics in the above-mentioned sense. Because of this, apparently, many scientists conclude that an idea crisis exists in fracture mechanics at the current stage of its development. Note also that the second area in classical mechanics may serve as the first stage in the study of nonclassical fracture mechanics.

The following studies may be conditionally classed among the ***nonclassical problems of fracture mechanics***.

1. Study of new mechanisms of fracture that are not described within the framework of the above five concepts and approaches (under Conditions 1-3) with appropriate analysis and attempts to formulate new fracture criteria corresponding to the phenomena under consideration.
2. Study of certain classes of problems related to new mechanisms of fracture of materials and structural elements by invoking specially formulated fracture criteria.

As already mentioned, the above classification (into classical and nonclassical problems) is rather conventional and not always unambiguous. Nevertheless, this classification determines fairly well the orientation of studies and their novelty, which seems to be rather important for the end-point analysis. It should be also noted that the number of fracture mechanisms increases considerably if the material microstructure, which is described differently, is taken into account. This feature pertains to the fracture mechanics of composites whose microstructure is considered at various levels. Scientists who study nonclassical problems and fracture mechanisms apply rather approximate design models. Such approximate design models are applied to the analysis of fracture in the microstructure of composites. The application of approximate design models leads to significant errors and, in many cases, to qualitative differences. Hence, it is rather difficult to carry out a reliable analysis of nonclassical problems and fracture mechanisms using approximate models. Therefore, results obtained in studying nonclassical problems and fracture mechanisms on the basis of quite strict design models are of considerable value.

The results on *nonclassical problems and fracture mechanisms* that have been obtained by the author and his followers at the S. P. Timoshenko Institute of Mechanics of the National Academy of Sciences of Ukraine within the past thirty years are briefly described here. Primary attention is drawn to a qualitative analysis of the basic aspects of the problems under correct three-dimensional statement. The following seven problems and associated fracture mechanisms are considered quite regularly.

1. Fracture of composites compressed along reinforcing elements.
2. End--crush fracture of composites subject to compression.

3. Shredding fracture of composites stretched or compressed along the reinforcing elements.
4. Brittle fracture of cracked materials with initial (residual) stresses acting along the cracks.
5. Fracture under compression along parallel cracks.
6. Brittle fracture of cracked materials under dynamic loads (with contact interaction of the crack faces).
7. Fracture of thin-walled cracked bodies under tension with prebuckling.

It should be mentioned that results for Problems 1-3 pertain only to the fracture mechanics of composites, whose microstructure, as already mentioned, is described at various levels, and results for Problems 4--7 equally pertain to the fracture mechanics of composites and to the fracture mechanics of metals and alloys. Based on the terminology accepted here, Problems 1-3 are attributed to failure mechanics and Problems 4-7 to fracture mechanics.

Note that the following two features are characteristic of the studies made by the author and his disciples on the above-mentioned seven nonclassical problems of fracture mechanics (as compared with the studies of other authors).

1. The studies were carried out by invoking the most strict and exact formulations within the framework of the mechanics of deformable bodies. For example, the three-dimensional linearized theory of stability of deformable bodies and the three-dimensional equations of statics of deformable bodies were applied to the study of buckling and the stress-strain state respectively. This remark addresses Problems 1-6. As for Problem 7, the stringency of the formulation and methods of study is ensured by applying the two-dimensional linearized theory of stability of thin-walled structural elements.
2. Problems 1-3 were studied within the framework of both the continual approximation (the model of a homogeneous orthotropic body with reduced constants – a three-dimensional formulation) and the model of a piecewise-homogeneous medium (the three-dimensional equations for a filler and binder and continuity conditions at interfaces). It have to be noted that the indicated model of a piecewise-homogeneous medium (in a three-dimensional formulation) is the most strict and exact within the framework of the mechanics of deformable bodies as applied to composites. We can introduce some corrections (specification of results) only by considering other boundary conditions at interfaces and other constitutive equations for the filler and binder.

It should also be noted that the results in *nonclassical fracture mechanics and associated fracture mechanisms* obtained at the S. P. Timoshenko Institute of Mechanics of the National Academy of Sciences of Ukraine are reported in the collective four-volume (five-book) monograph (in Russian).

Professor **Oscar H. Ibarra, Santa Barbara, Blaise Pascal Medal in Computer Science**

In recognition of his outstanding contributions in several areas of computer science, including theory of computing, design and analysis of algorithms, computational complexity, parallel computing, VLSI computation, formal verification, and membrane computing.

Oscar H. Ibarra
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Oscar H. Ibarra received the B.S. degree in Electrical Engineering from the University of the Philippines and the M.S. and Ph.D. degrees, also in Electrical Engineering, from the University of California, Berkeley. He is a Professor and past Chair of the Department of Computer Science at the University of California, Santa Barbara. Previously, he was with the faculties of UC Berkeley and the University of Minnesota.

Professor Ibarra was awarded a John Simon Guggenheim Memorial Foundation Fellowship in 1984. He is a Fellow of the Association for Computing Machinery, the Institute of Electrical and Electronics Engineers, and the American Association for the Advancement of Science. In 2001, he received the IEEE Computer Society's Harry M. Goode Memorial Award. He was awarded an Invitational Fellowship for research by the Japan Society for the Promotion of Science in 2002. The University of the Philippines Alumni Association presented him a distinguished alumnus award as the 2003 Outstanding Professional in the field of Mathematics, Statistics, and Computer Science. He was elected a member of the European Academy of Sciences in 2003. He is listed in the Institute for Scientific Information (ISI) database of 230 Highly Cited Researchers in Computer Science. He is a recipient of a Nokia Visiting Fellowship and is currently visiting the University of Turku. He was recently awarded the 2007 Blaise Pascal Medal in Computer Science from the European Academy of Sciences. Professor Ibarra is the Editor-in-Chief of the International Journal of Foundations of Computer Science and serves on the editorial boards of several international journals.

During his 40 years in academia, Professor Ibarra's main research focus has been, and continues to be, in the foundations of computing. These include the design and analysis of algorithms, theory of computation, computational complexity, parallel computing, formal verification, and membrane computing. Highlights of his work are given below.

Fully Polynomial Time Approximation Schemes

Many computational problems that occur in practice are combinatorial in nature. Consider, for example, the *Hamiltonian Circuit Problem.* Here, we are given a directed graph with n nodes (the graph may represent a map with the nodes representing cities in Europe). The question is whether there is a path that starts and ends at some node s which visits each city exactly once. Clearly, there is an algorithm (procedure) to solve this problem – try all possible paths of length $n-1$ and check if there is one that satisfies the requirement. But the number of possible paths is $(n - 1)!$ Thus, the algorithm takes time (i.e., number of steps) that is exponential in n, in the worst case. Except for very small values of n, this algorithm is not feasible, since it takes an enormous amount of time to execute (e.g., an algorithm that runs in

2^{60} steps, where each step takes 1 microsecond to execute, will take 366 centuries to complete its run; one that runs in 3^{60} steps will take 1.3×10^{13} centuries).

Another example is the *Knapsack Problem:* Given is a set of n objects $\{O_1, ..., O_n\}$. Associated with each object O_i is a pair of positive integers (w_i, p_i) – the weight and profit of the object. Also given are positive integers P and W. Here the question is whether there is a subset of the objects such that the sum of their weights is no more than W, and the sum of their profits is at least P. Again, a brute force algorithm for this problem involves an exponential number of steps.

A problem that can be solved by an algorithm that runs in time polynomial in the "size", n, of the problem, i.e., n^k for some k, is considered tractable, especially if the k is small. At present there are no known polynomial-time algorithms for the problems above. These problems are called decision problems, as they involve only a 'yes' or 'no' answer. Many decision problems generalize to optimization problems. For example, in the Hamiltonian Circuit Problem, one can attach weights (distances) to the edges of the graph and ask for a Hamiltonian circuit (if one exists) with minimum total weight (= sum of the weights in the path). Similarly, in the Knapsack Problem, one can ask for a solution that achieves the maximum total profit. It turns out that for both these optimization problems, there is a polynomial time algorithm if and only if their corresponding decision problem has a polynomial time algorithm. This polynomial-time relationship between the decision problem version and optimization version is true for many combinatorial problems.

The problems above are combinatorial – a brute force (exhaustive) algorithm involves looking at all possible combinations, thus exponential; but no better algorithms, i.e., running in polynomial time, are known. These problems belong to a large class of problems called NP-hard problems. They have the property that if one can be solved in polynomial time, then all problems in the class can be solved in polynomial time.

NP-hard problems can be found in many diverse areas: scheduling, computational biology, DNA sequencing, databases, internet computing, logic, network design (e.g., routing, network flows), VLSI/CAD, memory management (storage/retrieval), mathematical programming (e.g. linear programming), program optimization (code generation), logic, graph theory, algebra and number theory, games and puzzles, software and hardware verification, molecular computing, etc.

It is generally accepted that NP-hard problems cannot be solved in polynomial time, i.e., they are most likely intractable. Whether or not this is indeed true is an important long-standing open problem in complexity theory.

One approach for coping with NP-hard problems is to develop approximation/heuristic algorithms that may only give suboptimal results but that run in polynomial time. For example, in the optimization version of the Knapsack Problem, one might be satisfied with a suboptimal algorithm (one that returns a solution which does not return the maximal profit but is guaranteed to within some error) that runs in polynomial time.

Professor Ibarra was the first to introduce a technique called *fully polynomial time approximation schemes* for NP-hard problems. He has developed fully polynomial time approximation algorithms for the Knapsack and other problems. While researchers were aware that certain NP-hard problems could be "approximately solved" by polynomial time algorithms, his discovery that some could be solved by a polynomial time algorithm that could guarantee as small a fractional error as desired was a breakthrough. This pioneering work motivated many researchers to investigate the existence of polynomial time approximation algorithms for various NP-hard problems that are of practical importance and theoretical interest. Fully polynomial time approximation schemes are now standard material in algorithm design.

Translational (Padding) Techniques

Classification of decision problems in terms of their time and space requirements is an important issue in machine-based complexity. Techniques (e.g., "diagonalization") for establishing tight time or space hierarchies in deterministic models of computing is well understood. No techniques are known for establishing tight hierarchies in nondeterministic models. A nondeterministic device is one that allows "guessing" in its computation. The computation is a tree of paths, and an input is said to be recognized if there is at least one path in the tree that leads to success (i.e., to a 'yes'). The length of the path (respectively., the space needed by the device to process the path) is the time (respectively, the space) requirement for the given input.

Professor Ibarra originated and popularized the *translational* or *padding* techniques in complexity theory and used these techniques to solve several problems that had eluded solution by other researchers. In particular, he has established tight complexity class hierarchies for nondeterministic space-bounded Turing machines. It turned out that the techniques are also useful in establishing tight hierarchies in terms of other resource measures for other models of computation. The techniques are widely used in complexity theory.

Verification/Analysis of Infinite-State Systems

Developing tools for software analysis and verification is a very active area of research with considerable academic as well as industrial interest. Building reliable information systems is among the most challenging goals in information technology. An essential approach to developing reliable systems is to formally specify requirements and (data and system) designs and to verify them, since it is very costly to fix an error in a specification once the system is built. Automatic verification techniques can be used in the early phases to eliminate mistakes in specifications. It may never be feasible to automatically verify an implementation of a large system. However, if the system is specified unambiguously during the design phase, it may be possible to automatically verify its specification or to at least analyze and test the specification using automatic verification techniques.

There has been significant progress in automated verification techniques for finite-state systems. One such technique, model checking, has been successfully applied to verification of hardware protocols. However, existing model checking techniques do not scale very well to large systems and they are limited to finite domains. There is also a big difference between hardware and software design in that while hardware designs are inherently finite-state, software designs are often idealized as infinite-state systems. Thus, a great deal of recent work is focused on developing techniques for verification of infinite-state systems. However, for infinite-state systems, a fundamental problem - the *decidability problem*[1] -should be addressed before any attempts are made to develop automatic verification procedures. It is well known that it is impossible to automatically verify whether an arithmetic program with two integer variables will halt. Therefore, a key aspect of the research on infinite-state system verification is to identify what kinds of practically important infinite-state models are decidable with respect to a particular set of properties.

Professor Ibarra's contributions are in the development of fundamental techniques for the analysis and verification of infinite-state systems. The techniques are suitable for information systems that are capable of handling large, even infinite, state spaces. He has investigated the use of automata-theoretic techniques for proving the decidability (and complexity) of verification queries on infinite-state systems by restricting the properties or the

[1] A problem is *solvable* if there exists an algorithm to solve it; otherwise, it is *unsolvable*. For a decision problem, we usually use the terms *decidable* and *undecidable*, instead.

systems that can be verified. This entailed developing new machine (automata) models that are more powerful than finite-state automata, but still have important decidable properties. These investigations can lead to new and more efficient verification techniques than those available previously because the verification algorithms would not rely on state-space enumerations.

Counter machines are considered a natural model for specifying reactive systems containing integer variables. They have also been found to have a close relationship to other popular models of infinite-state systems, such as timed automata. However, counter machines are undecidable for verification in general. Professor Ibarra has studied various restricted models of counter machines to obtain new decidable models and identify the boundary between decidability and undecidability. He has discovered surprisingly powerful tools that are very useful in showing the solvability of verification problems for several important new models of infinite-state systems. The fundamental technique is the use of *counting by reversal-bounded counters* in machines to show decidability and solvability. The technique has been shown to have a wide range of applications.

Automata Theory and Formal Languages

Professor Ibarra is regarded as one of the world's top researchers in automata theory and formal languages. His work in these areas are fundamental and influential. He has introduced important models of computation and characterized their computing power, closure and decision properties. The techniques he has developed for showing decidability and undecidability of various problems in automata theory, formal languages, programming languages are well known. In particular, he has established some of the strongest results known on the undecidable properties of programs and abstract machines. His proof techniques are deep and quite intricate. He has used, e.g., the undecidability of Hilbert's Tenth Problem to prove surprising results concerning decision questions (e.g., "equivalence" and "optimality") of straight-line programs.

Professor Ibarra's contributions in Presburger arithmetic/semilinear sets, including the connection between such sets and reversal-bounded counter machines, simple programs, and Diophantine equations, play important roles in a wide variety of areas, including formal verification (as described in the previous section), data bases, and membrane computing. The techniques he has developed lay a foundation upon which many subsequent results are built.

Membrane Computing

There has been a flurry of research activities in the area of membrane computing (a branch of molecular computing) initiated eight years ago. Membrane computing identifies an unconventional computing model, namely a P system, from natural phenomena of cell evolutions and chemical reactions. Due to the built-in nature of maximal parallelism inherent in the model, P systems have a great potential for implementing massively concurrent systems in an efficient way, once future bio-technology (or silicon-technology) gives way to practical bio-realization (or a chip-realization). A P system consists of a finite number of membranes, each of which contains a multiset of objects (symbols). The membranes are organized as a Venn diagram or a tree structure where one membrane may contain other membranes. The dynamics of the system is governed by a set of (biologically-motivated) rules associated with each membrane. Each rule specifies how objects evolve and move into neighboring membranes, how membranes can be created and dissolved.

Membrane Computing has been selected by the Institute for Scientific Information (ISI) as a fast "Emerging Research Front" in Computer Science.

Various models of P systems have been investigated and have been shown to be universal, i.e., Turing machine complete, even with a very small number of membranes (e.g., 1 or 2 membranes). However, very little work has been done on investigating P systems that are nonuniversal, due to the difficulty of analyzing such systems.

Professor Ibarra's contributions in this area presented the first investigation of nonuniversal P systems. In particular, he has looked at the question of whether there exists a model of P systems where the number of membranes induces an infinite hierarchy in its computational power, This question had been open since the beginnings of membrane computing. Professor Ibarra has provided a positive answer to this open problem, as well as solutions to other important problems and was awarded a prize at the Workshop on Membrane Computing in 2003. Subsequently, he has given important characterizations of the power and complexity of various models of P systems.

Parallel Computing

Parallel computing involves *splitting* a problem into several, say *n*, smaller subproblems of approximately the same size, *solving* the subproblems simultaneously using *n* processors, and then *merging* their solutions to obtain the solution to the original problem. The total computation time is then the sum of the maximal time to solve any of the subproblems plus the times for splitting and merging. Ideally, the speed-up obtained would be of the order *n*, although in practice, the speed up is usually less than this, because of the overheads of splitting and merging.

Professor Ibarra has developed highly efficient parallel algorithms for various problems on several parallel machines. In particular, he has developed an innovative approach to convert sequential algorithms into systolic (a parallel computer model) algorithms. The technique allows one to design an algorithm on a sequential device that can then be automatically translated into a very efficient systolic algorithm. This design methodology has been successfully applied to various problems (e.g., in scientific and engineering problems), including those that were previously thought to be too difficult to parallelize, and in many cases yielding algorithms more efficient and easily proved correct than those obtained by direct design. He has demonstrated the power of the technique by employing it as a tool in resolving some long-standing open problems in the theory of cellular arrays.

Concluding Remarks

Professor Ibarra continues to work in various areas of theoretical computer science. Over the years, he has inspired and motivated students to work in these areas as well. He has successfully supervised the Ph.D. theses of a large number of students, many of whom have gone on to establish successful careers in academia and industry.

Professor **Sven Erik Jørgensen, Copenhagen, Blaise Pascal Medal in Earth Sciences**

In recognition of his outstanding contributions in the fields of ecological modelling, management of ecosystems, ecosystem theory, ecological engineering and ecological thermodynamics. He is one of the few multidisciplinary researchers that has understood how to integrate several disciplines to solve ecological and environmental problems. Sven Erik Jørgensen has been able to integrate ecology (particularly systems ecology), with management and technological issues (ecological engineering) and thermodynamics and has developed ecological models as an integration tool.

Sven Erik Jørgensen
Copenhagen University
Environmental Chemistry
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Ecological Modelling and Ecosystem Theory

Introduction: Three Steps of Development

My research work falls into three steps: 1) pollution abatement methods, but the selection of the right method requires 2) development of ecological models, which to give a right ecological answer requires understanding of ecosystems and their reactions, leading to an 3) ecosystem theory. The two latter steps that have been research area for the last almost forty years are presented below.

Ecological Modelling

Ecological models enable an integration of all what we know about a problem for a specific ecosystem. It is therefore a powerful tool to understand and manage ecosystems. Development of ecological models took off in the early seventies and in 1975 I started the scientific journal Ecological Modelling. Today, the journal publishes 4000 pages per year and has a citation index of 1.88. Many models covering many combinations of environmental problems and ecosystems are available to day.

In the seventies, eutrophication models were particularly in focus. My research team developed a model based on many and frequent observations in a relatively small lake with a simple hydrology and only six month retention time of the lake. The model was challenged by testing a prognosis, based on a significant reduction in the phosphorus input to the lake. The comparison of the prognosis performed by the model with the observations was acceptable on the one hand. On the other hand, the phytoplankton and zooplankton species of the lake changed because other species were better fitted to the new situation of reduced phosphorus concentration. Phytoplankton changed from dominant green algae to dominant diatoms and zooplankton from dominant *bosmina* to dominant *daphnia magna*. It means that the structure and the properties of the species considered in the model were not any longer in accordance with the actual structure of the lake after one to two years. It raised obviously the question: how can we develop models that are able to account for the adaptation processes and the shifts in species composition? It was a question of being able to find the changes in the properties of the species, that would give a better survival under the prevailing but steadily changed conditions. It was necessary to translate Darwin's survival of the fittest into a quantifiable concept.

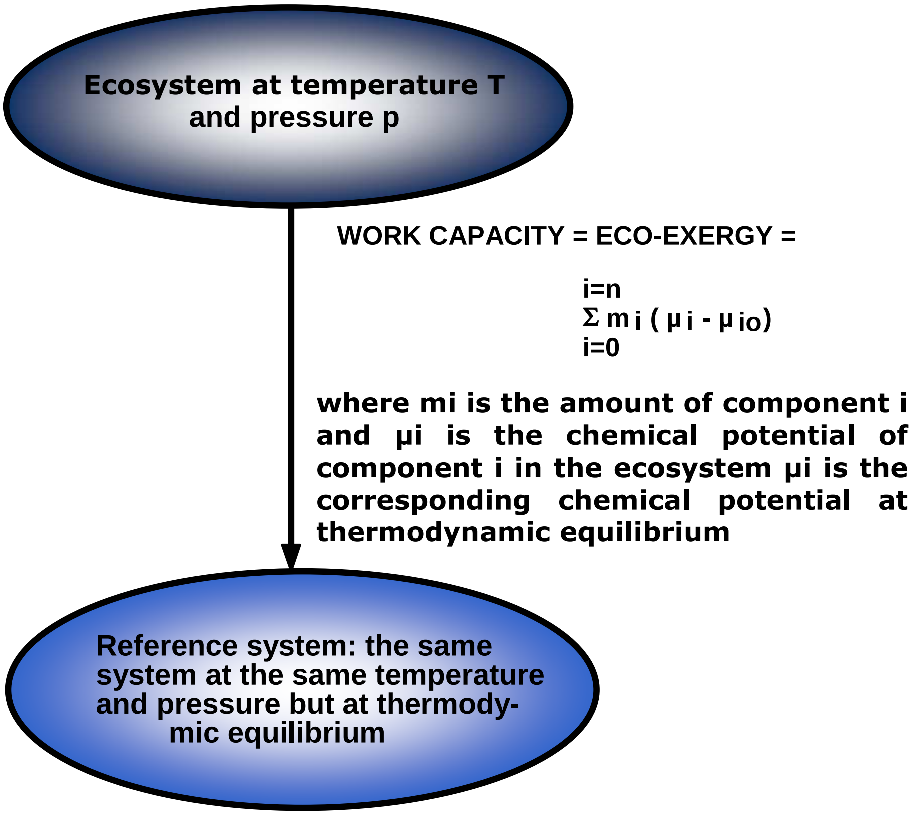

Figure 1. The eco-exergy content of the system is calculated in the text for the system relative to a reference environment of the same system at the same temperature and pressure but at thermodynamic equilibrium – it means an inorganic soup with no life, biological structure, information , gradients and organic molecules.

Eco-exergy; see Figure 1, was selected. It is the chemical energy that is contained in the many biochemical compounds in an ecosystem or rather in the model of the ecosystem.

The eco-exergy density = eco-exergy per unit of volume, can be calculated by the following equations:

$$Ex = \sum_{i=0}^{i=n} (\mu 1 - \mu 2)\ Ci = RT \sum_{i=0}^{i=n} Ci \ln Ci / Ci,o$$

$$B = \sum_{i=1}^{n} Ci \qquad pi = Ci / A$$

$$Ex = B\ RT \sum_{i=1}^{n} pi \ln pi / pio + B \ln B / Bo = BRTK,$$

- **where K is Kullbach's measure of information**

It *was* possible to develop models, that continuously follow the changes of the properties of the species, i.e. the model parameters, at a realistic rate. Eco-exergy was used to optimize the parameters, representing the properties of the dominant species: which set of parameters, i.e. the properties of the species, would give the highest eco-exergy, meaning the best survival? 18 different models of this type, denoted structurally dynamic models have been successfully developed up to day, meaning that they could describe the changes of the properties (= model parameters) in accordance with the actually observed changes. This development of structurally dynamic models opened for the possibilities to contribute to an ecosystem theory which was urgently needed to make theoretically short cut in ecological and environmental management.

Ecosystem Theory

The following hypothesis, which is a translation of Darwin to Thermodynamics, becomes a core of an ecosystem theory : **If a system receives an input of exergy, then it will utilize this exergy to perform work. The work performed is first applied to maintain the system (far) away from thermodynamic equilibrium whereby exergy is lost by transformation into heat at the temperature of the environment. If more exergy is available, then the system is moved further away from thermodynamic equilibrium, reflected in growth of gradients. If there is offered more than one pathway to depart from equilibrium, then the one yielding the highest eco-exergy storage (denoted Ex) will tend to be selected. Or expressed differently: Among the many ways for ecosystems to move away from thermodynamic equilibrium, the one maximizing dEx/dt under the prevailing conditions will have a propensity to be selected**

Strictly speaking eco-exergy is a measure of the useful work which can be performed. Conceptually, this obviously includes the energetic content of the material, i.e., biomass, but also the state of organization of the material. One way to measure the organization is the information content of the material, which could be the complexity at the genetic or ecosystem levels. Currently, the organizational aspect of exergy is expressed as shown above as Kullbach's measure of information based on the genetic complexity of the organism:

$$Ex = B\ RT\ K$$

where B is the biomass, R the gas constant, T the Kelvin temperature and K Kullbach's measure of information. The eco-exergy of the organism is found on basis of the information that the organism carries:

$$Ex_i = \beta_i b_i$$

where Ex_i is the exergy of the ith species, β_i is a weighting factor that consider the information the ith species is carrying in the biomass b_i

There are several supporting evidence to the hypothesis included of course the application of structurally dynamic models. Let us just mentioned two such illustrations:

The sequence of organic matter oxidation

The sequence of biological organic matter oxidation takes place in the following order: by oxygen, by nitrate, by manganese dioxide, by iron (III), by sulphate, and by carbon dioxide. This means that oxygen, if present, will always out compete nitrate which will out compete manganese dioxide, and so on. The amount of exergy stored as a result of an oxidation process is measured by the available kJ/mole of electrons which determines the number of adenosine triphosphate molecules (ATP's) formed. ATP represents an exergy storage of 42 kJ per mole. Usable energy as exergy in ATP's decreases in the same sequence as indicated above. This is as expected if the exergy storage hypothesis were valid (Table 1). If more oxidizing agents are offered to a system, the one giving the highest storage of free energy will be selected.

Table 1

Yields of kJ and ATP's per mole of electrons, corresponding to 0.25 moles of CH_2O oxidized (carbohydrates). The released energy is available to build ATP for various oxidation processes of organic matter at pH = 7.0 and 25 ˚C.

Reaction	kJ/mole e–	ATP's/mole e–
$CH_2O + O_2 = CO_2 + H_2O$	125	2.98
$CH_2O + 0.8\ NO_3^- + 0.8\ H^+ = CO_2 + 0.4\ N_2 + 1.4\ H_2$	119	2.83
$CH_2O + 2\ MnO_2 + H^+ = CO_2 + 2\ Mn^{2+} + 3\ H_2O$	85	2.02
$CH_2O + 4\ FeOOH + 8\ H^+ = CO_2 + 7\ H_2O + Fe^{2+}$	27	0.64
$CH_2O + 0.5\ SO_4^{2-} + 0.5\ H^+ = CO_2 + 0.5\ HS^- + H_2O$	26	0.62
$CH_2O + 0.5\ CO_2 = CO_2 + 0.5\ CH_4$	23	0.55

In Table 1, the first (aerobic) reaction will always out compete the others because it gives the highest yield of stored eco-exergy. The last (anaerobic) reaction produces methane; this is a less complete oxidation than the first because methane has a greater eco-exergy content than water.

Formation of organic matter in the primeval atmosphere

Numerous experiments have been performed to imitate the formation of organic matter in the primeval atmosphere on earth 4 billion years ago. Energy from various sources were sent through a gas mixture of carbon dioxide, ammonia, and methane. There are obviously many pathways to utilize the energy sent through simple gas mixtures, but mainly those forming compounds with rather large free energies (amino acids and RNA-like molecules with high eco-exergy storage, decomposed when the compounds are oxidized again to carbon dioxide, ammonia and methane) will form an appreciable part of the mixture.

Recently, it has been possible with the contribution from 8 other authors to present an ecosystem theory based on seven properties of ecosystems: 1) Ecosystems are physically open

2) Ecosystems are hierarchical systems 3) Ecosystems are ontic open 4) Ecosystems have directionality 5) Ecosystems are connected in synergistic networks 6) Ecosystems have a complex dynamics for growth and development 7) Ecosystems have a complex dynamics for meeting disturbances. 6) and 7) are mainly based on the hypothesis presented above. It has been possible to show, that many ecological rules can be explained as a consequence of this ecosystem theory.

Conclusion

Ecological modelling is to day a widely used tool in research and environmental management. Many ecological models have been developed over the last decades and the field is still growing very rapidly. The use of models is supported to day by an ecosystem theory and models are supporting a recently developed and useful ecosystem theory. We do have an ecosystem theory but we need to apply it more widely.

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Professor **Edward Layer, Cracow, Blaise Pascal Medal in Physics**

In recognition of his outstanding personal contribution to metrology of dynamical systems. Prof. Layer has made seminal contribution in elaboration of the general calibration theory of measuring systems intended for measurement of dynamic signals. Practical application of this theory create the basis for determining dynamic accuracy classes of different measurement systems applied in many scientific fields e.g. in electrical metrology, geodesy, diagnostic systems in medicine , meteorology and others, for which dynamic accuracy is not given by the producers and for which the method of such accuracy determination has not been worked out so far.

Edward Layer
Cracow University of Technology
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Poland

Basic Problems of the Measuring Systems Calibration Intended for Dynamic Measurements

Although we might not realize it we are constantly required to perform a whole variety of measurements. When shopping we weigh or measure the products that we are interested in, or buy products that have already been weighed or measured for us, when stopping at a petrol station we check our tyre pressure and make a note of how much petrol we have refuelled to our tank. In the morning we might check the outside temperature using a thermometer and possibly consult a barometer to determine the atmospheric pressure. In our homes various meters record the amount of electricity, gas or water that we are using. Obviously in laboratories, scientists, engineers and technicians perform measurements in the fields of physics, chemistry, biology etc. that are much more complicated and involved. The common feature of all these measurements however is that we never query their validity. We go further even, and regard the measurements as being totally error free. This of course cannot be true as there is no such thing as an error free measurement and any measurement will always carry with it a margin of error. This error might be bigger or smaller depending on the certified level of accuracy of the device that is used to perform the measurement. The certified level of accuracy determines the maximum error that can be expected at any point of the measuring instrument’s range and is verified using calibration processes laid down by international regulations which are controlled in each country by the corresponding weights and measurements office. These regulations cover the hierarchy of standards, the calibration circuits and valid calibrating procedures. The class index resulting from the value of the maximum static errors constitutes a basic criterion for the estimation of metrological quality for such instruments. It determines the classification of the calibrated instrument at an adequate level in the hierarchy of its accuracy. Mathematical methods for static error calculation and calibrating procedures for instruments intended for static measurements are well established and have been available for a long time.

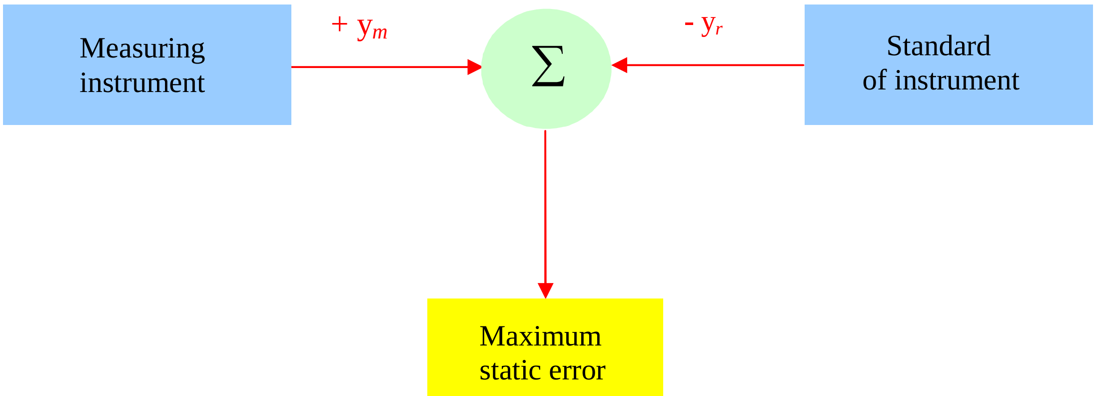

Fig.1. Block diagram for calibration of measuring systems intended for static measurements

Things are very different in the case of measuring systems for dynamic measurements for which the input signal is time dependent, of arbitrary shape and impossible to predict, as for example, signals originating from seismic waves, signals of acoustic pressure generated by explosions of explosive charges, signals from earth crust vibrations caused by earthquakes, etc. Fig.2 presents exemplary dynamic signals.

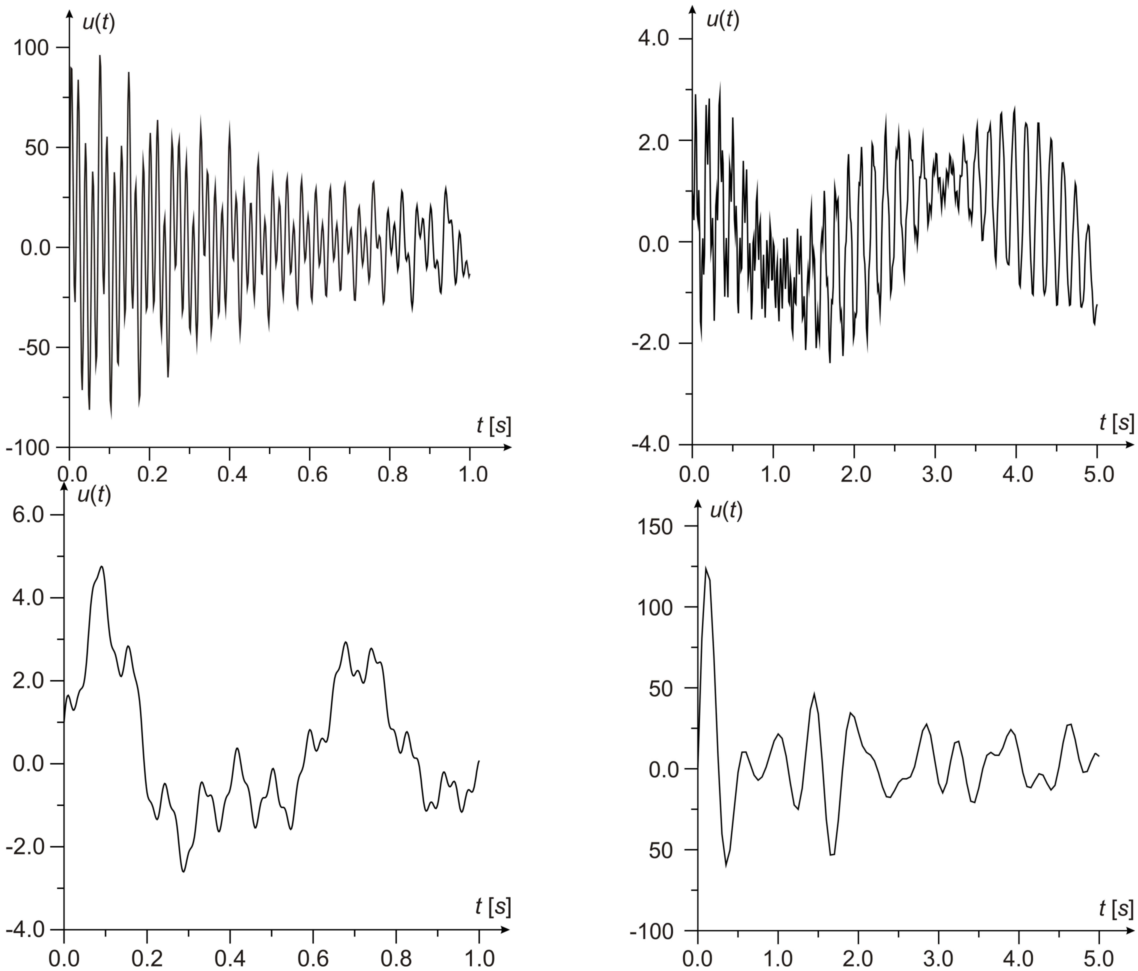

Fig.2. Exemplary shapes of dynamic signals

For systems of this type neither legal regulations concerning calibration nor specific calibration procedures have been worked out so far. Consequently, neither dynamic accuracy classes nor the accuracy hierarchies based on them have been determined for these systems. The reason for this is that the determination of errors is possible only if the input signal used for their calculation is known. As it is impossible to analyze the full set of all imaginable input dynamic signals we need to limit the signals considered. The question immediately arises: what signals should we use for the calibration of systems which have at their input dynamic signals of unknown shape and unknown spectral distribution. A solution to this question is to consider the signal that maximizes the errors. The great merit of using such a signal is that results can be mutually compared regardless of the measured signal's shape as much as the errors determined will always be greater or, at least, equal to the value resulting from a signal of any shape which could appear at the input of the system. Effectively all the possible input signals to a real system are taken into consideration at the same time. Therefore the value of maximum errors can create the basis for the hierarchy of dynamic accuracy, just like class indexes create the basis for hierarchies of accuracy of the instruments applied for static measurements.

Analyzing the solutions for deriving the maximum error for the calibration of instruments intended for static measurements it became apparent that just as in the case of static measurements the key to answering the question posed above was to consider maximum errors which could be achieved by using special signals, maximizing assumed error criterion.

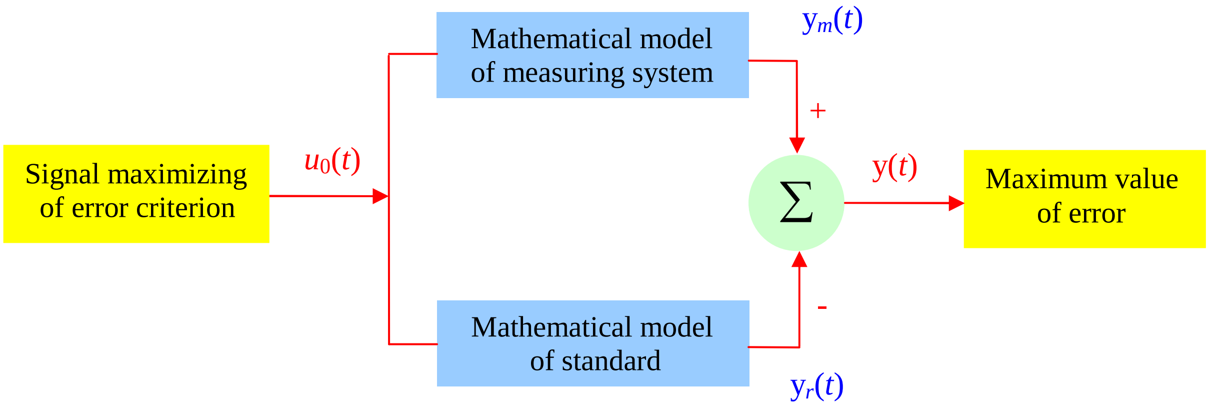

Fig.3. Block diagram for calibration of measuring systems intended for dynamic measurements

The procedure of maximum error determination needs, however, to provide a solution of many problems such as:

- determination of the mathematical models of the calibrated systems and their standards,
- adoption of the error criterions,
- determination of the constraints which should be imposed on the calibrating signals in order to match their dynamics to the dynamic properties of the calibrated systems,
- proving that signals with imposed constraints exist and that they are attainable,
- determination of signal shapes with constraints imposed,
- developing a computer program for the calculation of errors generated by these signals,

- calculation of the maximum errors,
- setting the hierarchy of dynamic accuracy for calibrated systems.

In order to determine mathematical model of calibrated system we can apply many different computer programmes based on the identification methods e.g. Matlab, Lab-View, Mathcad. However for calibration procedure the most convenient is to denote the model by means of differential equations, state equations or transfer functions. Using methods related to the Maclaurin series result in very accurate models. These methods ensure that mapping of the models is almost perfect at the beginning of the time interval, which is of particular importance in cases of the system models whose rated operation regime is a dynamic mode far away from a steady state. Special mathematical transformations were developed for the conversion of the coefficients of exponential series into corresponding coefficients of the differential equations and the main advantage of these transformations was the possibility of obtaining an arbitrarily high convergence of models.

Up to now, regulations governing the selection of standards for dynamic measuring systems have not been developed. This is a consequence of the fact that these standards present different objective functions. In such cases mathematical model of standards are usually presented as a simple mathematical record of the function the calibrated systems are to meet. Because of this reason mathematical model of standards are not to difficult for determination.

With regard to the selection of error criteria, our choice is very limited. The criteria used here are most often defined in C space as an absolute error or in L^2 space as the integral square error and very similar to this, the mean-square-error. Sometimes time as a weight function is introduced to the error presented in L^2 space. In engineering practice the most commonly used are the integral square error criterion and absolute error criterion.

Different constraints can be imposed on the signal maximizing chosen error criterion. Obviously a magnitude constraint must always be applied. Additionally in order to match the dynamics of the calibrating signals to the dynamics of physically existing calibrated systems, since they can only transmit signals with limited value of rate of change, further constrain should be taken into consideration. Proper matching is obtained by restricting the maximum rate of change of the calibrating signal to a value less or at most equal to the maximum rate of the step response of the system. The same constraint can be also determined using the frequency characteristic of the calibrated system on the base of the maximum angular frequency. This maximum corresponds to the cut-off frequency of this characteristic which can, but does not need, to meet a 3dB reduction in its magnitude.

Having mathematical models of calibrated system and its standard, chosen error criterion and having determined constraints which should be imposed on the calibrating signal we can approach the most difficult part of our task, namely the determination of the signal maximizing the chosen type of error. For this purpose we have to:

- point out the mathematical proof that signal with imposed constraints exists,
- determine the space where this signal exists and to find, if possible, an analytical solution with respect to this shape,
- derive a formula describing the maximum value of the error resulting from the determined signal,
- develop algorithm and computer program to calculate the error we were looking for.

The determined error is function of time, which occurs in upper limit of integration for errors defined in L^2 space or in fixed time interval for errors defined in C space. Changing in process of calculation this value of time up to setting time of system we can determine the full characteristic of maximum error. This characteristic constitutes the base for establishing the hierarchy of accuracy of calibrated system.

Setting up the hierarchy of accuracy for systems intended for the measurement of the same dynamic quantities on the base of the full characteristic of maximum errors requires determining the interval of the possible errors for the full set of the same type systems (e.g. strain gauge amplifiers, accelerometers, electroencephalographs, etc). The division of this interval into some subintervals will create the corresponding levels of such a hierarchy. Determining the hierarchy levels will require extensive coordination and consultation between the various metrological centres and producers of measuring systems, as up to now these have not been established and all the proposals in this field will be present quite new solutions.

Example

As an example mathematical proof of the existence and attainability of signal maximizing integral square error criterion with two constraints imposed on it has been presented below.

1. General assumption

Let the mathematical model of a measuring system be given by state equation

$$\begin{aligned} &\dot{x}_m(t) = A_m x(t) + B_m u(t) \qquad x_m(0) = 0 \\ &y_m(t) = C_m^T x(t) \end{aligned} \tag{1.1}$$

and let the system constituting its standard be given by a similar equation

$$\begin{aligned} &\dot{x}_r(t) = A_r x(t) + B_r u(t) \qquad x_r(0) = 0 \\ &y_r(t) = C_r^T x(t) \end{aligned} \tag{1.2}$$

Let us introduce a new state equation

$$\begin{aligned} &\dot{x}(t) = Ax(t) + Bu(t) \\ &y(t) = C^T x(t) \end{aligned} \tag{1.3}$$

in which

$$x(t) = \begin{bmatrix} x_r(t) \\ x_m(t) \end{bmatrix} \quad A = \begin{bmatrix} A_r & 0 \\ 0 & A_m \end{bmatrix} \quad B = \begin{bmatrix} B_r \\ B_m \end{bmatrix} \quad C = \begin{bmatrix} C_r \\ -C_m \end{bmatrix} \tag{1.4}$$

where in (1.1)-(1.4) $u(t)$ and $y(t)$ are input and output respectively, $x(t)$ is state vector, A, B, C are real matrices of corresponding dimensions.

2. Existence and attainability of signal

Let us assume that U is the set of signals $u(t)$ segmentarily C^1 over the interval [0,T], and the error $y(t)$ of the measuring system relative to its standard is expressed by inner product

$$I(u) = \int_0^T [y(t)]^2 dt = (Ku, Ku) \qquad u \in U \tag{2.1}$$

where

$$Ku = y(t) = \int_0^t k(t-\tau)u(\tau)d\tau \tag{2.2}$$

and

$$k(t) = C^T e^{At} B \quad (2.3)$$

Let us consider the signal $h \in U$ and let the following condition be fulfilled

$$\forall\, 0 < \mathrm{b} < \mathrm{c} < \mathrm{T} \quad \exists\, h \in U : supp\ h \subset [\mathrm{b,c}] \quad (2.4)$$

and positive square error

$$I(h) > 0 \quad (2.5)$$

Let us define the following set A of signals with imposed constraints of magnitude a and rate of change ϑ

$$A := \{\, u(t) \in U : \ |u(t)| \le a,\ |\dot{u}_+(t)| \le \vartheta,\ |\dot{u}_-(t)| \le \vartheta,\ t \in [0,T]\} \quad (2.6)$$

where $\dot{u}_+(t)$ and $\dot{u}_-(t)$ are increasing and decreasing derivative of $u(t)$ respectively.

Let $u_0(t) \in A$ fulfill the condition

$$I(u_0) = sup\{I(u):\ u \in A\} \quad (2.7)$$

Theorem

$$\forall\, t \in [0,T] \ \ |u_0(t)| = a \ \text{ or } |\dot{u}_{0+}(t)| = \vartheta \ \text{ or } |\dot{u}_{0-}(t)| = \vartheta \quad (2.8)$$

Proof

Suppose that (2.8) is not true. Then

$$\exists \varepsilon > 0, \quad \exists\ 0 < \mathrm{b} < \mathrm{c} < \mathrm{T} \quad (2.9)$$

such, that

$$|u_0(t)| \le a - \varepsilon, \quad |\dot{u}_{0+}(t)| \le \vartheta - \varepsilon, \quad |\dot{u}_{0-}(t)| \le \vartheta - \varepsilon, \quad t \in (\mathrm{b,c}) \quad (2.10)$$

Let us choose h according to (2.4)

$$supp\ h \subset [\mathrm{b,c}], \quad I(h) > 0 \quad (2.11)$$

then for small $d \in \Re$, say $d \in (-\delta, \delta)$ is

$$u_0 + dh \in A \qquad \forall\ d \in (-\delta, \delta) \quad (2.12)$$

and from the optimum condition $u_0(t)$ it results that

$$I(u_0) \ge I(u_0 + dh) \quad (2.13)$$

hence

$$I(u_0) \ge I(u_0) + d^2 I(h) + 2d(Ku_0, Kh) \qquad d \in (-\delta, \delta) \quad (2.14)$$

and

$$0 \ge d^2 I(h) + 2d(Ku_0, Kh) \qquad d \in (-\delta, \delta) \quad (2.15)$$

However, the last inequality will never be fulfilled for $I(h) > 0$, $d \in (-\delta, \delta)$. So, from this contradiction it easily results that $I(u_0)$ can fulfil condition (2.7) if input signal $u_0(t)$ reaches one of the constraints given in (2.8).

Corollary

The proof presented above reduces the shape of the $u_0(t)$ signals to triangles or trapezoids if constraints of magnitude and rate of change are imposed simultaneously. It means that signals u_0(t) can only take the form of triangles with the slope inclination $|\dot{u}_{0+}(t)| = \vartheta$ or $|\dot{u}_{0-}(t)| = \vartheta$ or of trapezoids with the slopes $|\dot{u}_{0+}(t)| = \vartheta$ and $|\dot{u}_{0-}(t)| = \vartheta$ and a magnitude of a.

Carrying out the proof in an identical way, it can be shown that if only one of the constraints is imposed to the signal, either of magnitude a or of the rate of change ϑ, then the error $I(u_0)$ reaches maximum if the signal reaches this constraint over the interval [0, T].