Mathematical and computational modeling in Mexico

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I want to thank Professor Mario Suarez for having invited me to write this Introductory Chapter, whose initial intention was to give a historical background of Mathematical and Computational Modeling (MMC) in Mexico. However, I must confess that in order to give a fair and balanced account of the past and present state of MMC a very thorough study and research would be required. This, however, is beyond the available time and resources. Thus, the scope of this Chapter was severely limited. It only contains a rather schematic and general historical perspective, together with a few examples, drawn from my own personal experience, of the MMC activities that have been carried out in Mexico up to now. We hope these examples will be useful as illustrations of what has been done so far, but the resulting picture is far from representing an integrated and fair image of the MMC activity in Mexico. In particular, there are many people working in MMC whose work deserves attention and are not here included; my apologies to them all.

WHAT IS MMC?

Predicting nature's behavior is an ancestral human aspiration. For this purpose, our forefathers used supra-natural means, including magical and religious thinking. However, throughout history, this ambition of mankind has been a basic motivation for science development. It actually took a considerable time-span, but eventually it was recognized that scientific means were the most effective ones for performing nature-behavior prediction and that in turn "scientific prediction" required deep knowledge of nature and its phenomena. Furthermore, it must be pointed out that scientific and technological knowledge by itself is not enough for predicting the behavior of nature, and of other systems that are important to humans, since behavior prediction requires integrating such knowledge into models capable of mimicking those systems. In addition, it was also eventually recognized that the most effective models are mathematical models. Newton, in the XVII Century, was the pioneer and founder of such school of thought when he developed the required mathematical methods and illustrated its power by successfully modeling the Planetary System's motion. This awoke the consciousness of his contemporaries of the potential of mathematical modeling and stimulated further expansion of his basic concepts.

Newton was followed by many generations of physicists and mathematicians, who developed his ideas and applied them to an amazing diversity of systems in science and engineering. As far as continuous macroscopic systems are concerned –among which most engineering systems are included-, the theoretical framework was crowned by the axiomatic formulation developed during the XX Century, under the leadership of Truesdell, Noll and others [1, 2]. Such a theoretical framework was very impressive, albeit insufficient because although its range of applicability included practically all systems of interest, the analytical tools available were very limited and only capable of dealing with simple systems –linearity of the models was an ever-present assumption and even so, simple geometry and simple properties were always required-, and not suitable for supplying the detailed information that is needed in many scientific and engineering applications. When that was the state of the art, the usefulness of mathematical modeling as an engineering tool was severely hampered. However, that situation sharply changed during the second half of the XX Century with the advent of electronic computing. Nowadays mathematical and computational modeling is the most efficient method for integrating scientific and technological knowledge, with the purpose of performing effectively scientific prediction.

Science and engineering in ancient Mexico

Indigenous scientific development in Mexico was quite significant. Autochthonous advances in Astronomy and Mathematics are proverbial, but also advances in hydraulics and engineering were outstanding, although not as well known [3,4]. In the VIII Century, in the time when Teotihuacán culture flourished, irrigation was based on the use of springs. Later on, the water of the lake in which Tenochtilán -the ancient Aztec capital on the site of present-day Mexico City- was located was salty and unsuited for human consumption. However, in the Valley of Mexico springs were abundant and the fresh water they used to produce was a valuable source for water supply of the people that lived on it. Thus, large aqueducts were constructed; among them, one carried the water from Chapultepec springs, and one more from Coyoacán springs. It is also known that the works used for supplying water to Texcoco were built by Nezahualcóyotl: legendary king, poet and engineer.

On the other hand, through history the cities located in the Valley of Mexico have been susceptible to flooding during the annual rainy season. To diminish such risks and reduce the damages, the Aztecs built boulevards, ditches and other hydraulic works, dividing with them the waters into sectors and controlling in this manner the water flow. The Nezahualcóyotl ditch is especially famous and used to go from the North to the South of the Valley of Mexico.

Mexico's scientific renaissance

That not withstanding, contemporary scientific and engineering activity of Mexico actually started after the 1910 Mexican Revolution. Political stability was reestablished in the 1930's, and at the end of that decade and beginning of the next one, the foundations of contemporary scientific development were laid down. Nationalism, one of the revolutionary-ideology's components, included the idea that a new nation had to be built and that in this endeavors every Mexican citizen should participate. Social demands, as well as a thorough revision of the material needs, required for the modernization of the country, also had an important bearing in the pos-revolutionary governmental programs. The "Comisión Nacional de Caminos" (the National Roads Commission) was created in the twenties of the XX Century, as a governmental agency in charge of an ambitious road construction program that just then started. Similarly, the "Comisión Nacional de Irrigación" (the National Irrigation Commission) was also created. This latter commission eventually became the "Secretaría de Recursos Hidráulicos" with visible responsibilities in dam construction and dam operation, while the "Comisión Nacional de Caminos" became the "Secretaría de Obras Públicas", with responsibilities in roads and also dams construction. Furthermore, the oil industry was nationalized in 1938 and the enterprise "Petróleos Mexicanos" that has been in charge of its administration ever since, was established. Safe water supply for the population and the emerging activities, together the need to generate electricity so much required for the modernization of the country, soon led to a boom in road building and construction of other public works such as dams. A nationalistic private sector also played an important role in these developments. In the 1940's, a group of distinguished, and then young, Mexican engineers created what eventually became a very important construction enterprise; namely, "Ingenieros Civiles Asociados", ICA, that was instrumental in carrying out many of the governmental projects. The "Golden Age" of Mexican Engineering (especially Civil Engineering) that thrived during the 1940's and extended over many decades after, must of course be attributed to the needs created by the above mentioned boom in public works, but ICA was the main catalyst of it. In the chemical industrial sector Bufete Industrial played a similar role. In summary, the Mexican Revolution of 1910 created a new consciousness of social needs and aspirations, which in turn gestated many new activities that in turn generated a boom of engineering activities; but the chain reaction did not end there, because the demand of engineering professionals in turn soon stimulated engineering teaching, engineering teaching pushed science teaching, and science teaching pushed science research. It was then when the precursors of present-day research institutions were established.

The ancestral "Real y Pontificia Universidad de la Nueva España", which was founded in 1551 and was reopened in the XX Century as the "Universidad Nacional de México", became today's "Universidad Nacional Autónoma de México" (UNAM) in 1929, when it achieved autonomy. UNAM played a central role in the initiation of research activities in Contemporary Mexico. Most of the civil engineers needed in the pos-revolutionary Mexico, including ICA's engineers, were trained at the "Escuela Nacional de Ingenieros", the UNAM's Facultad de Ingeniería of today, while petroleum engineers and geologists were educated at the recently created Instituto Politécnico Nacional (IPN). Furthermore, the Escuela Nacional de Ingenieros was the womb in which the present day research institutions in engineering and hard sciences (Physics and Mathematics) were gestated. As for Chemistry, a corresponding role was played by the "Escuela Nacional de Ciencias Químicas". Teaching of pure sciences began at the "Facultad de Ciencias", created in 1939 within the Escuela Nacional de Ingenieros, and in the 1939-1950 period the institutes of basic research on Mathematics, Physics, Geophysics, Chemistry and Astronomy were established. The "Mexican School of Thought" in Physics and Mathematics owes much to some Ivy League universities, particularly Princeton. And in this, the personality of Solomon Lefchetz should be mentioned. On the other hand, some of the most distinguished applied mathematicians in Mexico were trained at Brown University.

Those developments not withstanding, most of the activities on mathematical and computational modeling (MMC) were associated with the specific endeavors related with engineering work and certain number of applied research institutions were created. With ICA as its main promoter, the Instituto de Ingeniería was created in 1956, within the Facultad de Ingeniería. The first computer devoted to research, a 650 IBM, was installed at the "Facultad de Ciencias" in 1958. Other institutes of applied research and development were the Instituto de Investigaciones Eléctricas, the Instituto Mexicano del

Petróleo and the Instituto Mexicano de Tecnología del Agua, established in 1962, 1966 and 1981, respectively.

Sampling MMC in Mexico

The Pacific Volcanic Rim limits a large part of the Mexican territory, on the west coast; furthermore, the Mexican Trans Volcanic Belt goes across the country, from the Pacific Ocean to the Gulf of Mexico. Seismicity is high in Mexico, so that the observation and study of earthquakes, and their effects, have had high priority since the beginning of the XX Century. The National Seismological Service was established in 1910 and has been in charge of the Institute of Geophysics since this latter institute was established in 1949.

Mexico, together with USA, Japan and a few other countries, was pioneer in the study, research and application of Seismic Engineering, also called Earthquake Engineering. In Mexico, a very strong and still highly respected Seismic Engineering research group was created under Emilio Rosenblueth's leadership. Rosenblueth, whose friendship I enjoyed until his death in 1994, was a worldwide leader, pioneer and founder, together with Newmark, of Earthquake Engineering as an engineering discipline [5]. One of the main objectives of Seismic Engineering is to predict, combining both deterministic and statistical models, the occurrence and the effects, especially on civil engineering structures, of earthquakes. So, MMC is a very fundamental tool in this area of engineering. Models that have been built in Mexico include statistical models for predicting the probability of occurrence of earthquakes, including time and location, magnitude and other features such as its predominant period [6, 7]; models of the focal behavior of earthquakes; effect of the structure of the crust and upper mantle into the transmission of the elastic waves from the seism focus to the structure location; the effect of the local geology into the characteristics of the motion that excites the engineering structure under study; soil-structure interaction models that take into account the effect of the structure into the soil motion; deterministic models for predicting the response of different engineering structures such as buildings and dams, when the motion that excites them is known; and models of the stochastic processes that perform the structures that are governed by differential equations of the Fokker-Plank type [8].

The results of all this research has been very useful not only in Mexico but in many other parts of the world. Mexican experts in Earthquake Engineering, such as Luis Esteva, have to travel to many other seismic countries to advise local experts due the high prestige of the Mexican earthquake-engineering institutions. The research results that have been obtained in this area have been incorporated in building regulations not only of Mexico City, but of many other cities of the world. This has been a great contribution to the safety of the people and their material possessions.

For a time, long ago, the author of this Chapter was an active participant of the Earthquake Engineering research group and at that time he also did some research on Seismology, which deals less directly with practical problems, but the new knowledge generated by it, is rapidly incorporated by disciplines with a more practical orientation such as Seismic Engineering. Many of such studies are carried out with the purpose of establishing the physics and structure of the Earth interior. One of the main tools used for this purpose are models of the elastic motion in the crust, mantle and deep interior. So, frequently such a kind of research also investigates basic properties of elastic motion. During a time there was worldwide interest in establishing the distribution on the Earth of the upper mantle and including features such as its thickness. Besides some deep drilling projects, which were very costly, MMC models of elastic surface-waves -mainly Love and Rayleigh waves- were used for this purpose. Mexico participated through the Gulf of California Project that was carried out in collaboration with the University of California, at Los Angeles (UCLA). Among the results of that project that were obtained in Mexico and should be cited, is the derivation of orthogonality relations for Rayleigh waves. Orthogonality relations for Love waves had been known for a long time, but for Rayleigh waves they were not known until 1964 [9].

One of our most important problems is securing the everyday water supply throughout our large country and the best way of coping with it is through scientific management of our resources [10], which requires a great variety of mathematical and computational models; models of surface waters and models of ground water. In the case of the former, water flow -including flood prediction- and contaminant transport in rivers and channels, deterministic and statistical modeling of basin response, dam design, to cite a few. Flood prediction, for example, is essential for the design of bridges and requires the modeling of the basin response. The administration of groundwater also puts very important challenges in the modeling of subsurface water flow and contaminant transport. On the other hand, urbanization is a reality of our changing world that is causing the birth and growth of many megalopolises. A central question is "how can our cities be sustained under these circumstances?" And the Mexico City Metropolitan Area (MCMA) exemplifies, to an extreme degree, these problems [3, 4]. There, a very important problem is land subsidence, which is induced by the severe pumping of the aquifer, due to the leaky character of the subsurface hydrologic system.

In Mexico, modeling of surface water systems has being going on for a long time, at least since the 1950's. The leader who organized a very prestigious group in this area was the former José Luis Sánchez Bribiesca. Many of the most distinguished Mexican hydrologists of today were his students; to cite just one: Álvaro Aldama, who was not only a former general director of IMTA, but the very one that consolidated that national institute.

As for groundwater, it would be difficult to overstate its importance for a country at which more than 60% of its territory is arid or semiarid. A pioneer and worldwide leader of the application of MMC to groundwater is George F. Pinder; first at the US Geological Survey (USGS) and later at Princeton University. In Mexico, scientific research of groundwater using mathematical and computational models was initiated in the late sixties at the Institute of Geophysics under Herrera's leadership [11, 12]. Later, he was invited to join the Advisory Council at Princeton and since then Herrera and Pinder have had a very fruitful collaboration. The main scientific contribution to the mathematical modeling of groundwater made by Herrera and his collaborators at UNAM, was the invention and development of the "Integro-differential equations approach to leaky aquifers" [13-15], sometimes called "Herrera's Integrodifferential Equations Approach to Leaky Aquifers". Thereby, it should be mentioned that the subsurface hydrologic system of Mexico City is precisely a multilayered leaky aquifer system. The software developed by the USGS in 1994 [16], is based on Herrera's approach. Because of his pioneering results, Herrera has been considered to be founder – together with Neumann and Witherspoon- of the "Multilayered Aquifer Systems Theory" [17]. Mathematical and computational models were developed for the construction of the artificial lakes at the Texcoco Basin [18], the subsurface hydrologic system of Mexico City (actually, the MCMA system) [19, 20] and the geothermal systems of Cerro Prieto, B.C., and Los Azufres, Mich. Nowadays, MCM models are used routinely in Mexico to deal with many groundwater problems, albeit there is a shortage of professionals and engineers adequately trained in subsurface hydrology.

As for basic contributions to the methodology of MMC, probably the most conspicuous group doing research in that area is the "Grupo de Modelación Matemática y Computacional" del Instituto de Geofísica, UNAM [21-43], whose leader is also Editor and founder of the International Journal: "Numerical Methods for Partial Differential Equations", published by Wiley (New York) since 1985. Many of its research themes stem from an "Algebraic Theory of Boundary Value Problems" for partial differential equations, and the "Theory of Partial Differential Equations on Discontinuous Piecewise-Defined Functions" that derived from it. The algebraic theory has been developed through a long time span [21-43]. It identifies and makes extensive use of some algebraic properties of boundary value problems. In the first part of its development, the research that originated it was oriented to construct a general framework for variational principles of boundary value problems that at the time were being extensively studied all over the world. This was the period of the initial stages of the application of computers to solving partial differential equations, and variational principles were the means used for disctretizing such equations. The theory that was so obtained accommodates practically all variational principles for boundary value problems known at such a time. Furthermore, it also encompasses Trefftz methods, bi-orthogonal systems of functions and a criterion for completeness of systems of functions (originally introduced as *C-completeness*, but later known as *T-completeness*, or *TH-completeness*). This theory also yields a suitable framework for the development of complete systems of solutions of partial differential equations (see [44], Ch. II, where the exposition is based on Herrera's *T-completeness* or *TH-completeness*, concept). Furthermore, according to Begehr and Gilbert _the algebraic theory supplies the basis for effectively applying to boundary value problems the function theoretic methods of partial differential equations. Indeed, in [44], p115, these authors assert:
'The function theoretic approach which was pioneered by Bergman and Vekua and then further developed by Colton, Gilbert, Kracht-Kreyszig and Lanckau and others, may now be effectively applied because of this result of the formulation by Herrera [21] as an effective means to solving boundary value problems'.

On the other hand, the algebraic theory has also been useful for establishing the theoretical foundations of *Trefftz methods*. This time the citation comes from J. Jirousek, one of the most conspicuous representatives of *Trefftz methods* [45, p324]: *'the mathematical foundations of which* –referring to Trefftz methods- *have been laid mainly by Herrera and co-workers'*. In 1984, the Pitman's Advanced Publishing Program collected many of the results of the theory in a book [21]. An important element of the theory of differential equations in discontinuous functions that was introduced by Herrera immediately afterwards, in 1985, is a kind of Green's formulas applicable to them and referred to as *Green-Herrera formulas*. They have played a central role in later developments. Their relevance is two-fold: firstly, they supply more explicit expressions for the distributional derivatives and, secondly, they extend the notion of distributional derivative in a way that permits applying *fully discontinuous trial and test functions* simultaneously, something that is not possible when the standard theory of distributions is used. Apparently, it had been this latter fact what had prevented, until recently, the development of more direct approaches to partial differential equations formulated in discontinuous piecewise-defined functions.

This more recent work-phase of the theory includes certain number of applications. Among them: the introduction of the *Localized Adjoint Method* (*LAM*) that in turn supplied the theoretical basis of the *Eulerian-Lagrangean LAM* (*ELLAM*), a numerical method that has had considerable success in treating advection-dominated transport; more advanced applications to Trefftz method and studies of several aspects of domain decomposition methods; and a general class of methods that are collectively denominated as *'finite elements methods with optimal functions (FEM-OF)'*. This latter kind of methods is more general than *LAM* and has yielded some very effective procedures for applying orthogonal collocation; also, for developing some classes of enhanced finite elements (see [43], in this volume).

A truly general and systematic theory of Finite Element Methods (FEM) should be formulated using, as *trial* and *test functions*, *piecewise-defined functions* that can be fully discontinuous across the *internal boundary* which separates the elements from each other. Some of the most relevant work addressing such formulations is contained in the literature on *discontinuous Galerkin (dG) methods* and on *Trefftz methods*. However, the formulations of partial differential equations in discontinuous functions used in both of those fields are indirect approaches, which are based on the use of *Lagrange multipliers* and *mixed methods*, in the case of *dG methods*, and *the frame*, in the case of *Trefftz method*. The "Theory of Partial Differential Equations on Discontinuous Piecewise-Defined Functions" [41] addresses this problem from a different point of view and formulates the partial differential equations in *discontinuous piecewise-defined functions*. Such an approach is more direct and systematic, and furthermore it avoids the use of *Lagrange multipliers* or a *frame*, while *mixed methods* are incorporated as particular cases of more general results implied by the theory. When boundary value problems are formulated in discontinuous functions, well-posed problems are *boundary value problems with prescribed jumps (BVPJ,)* in which the *boundary conditions* are complemented by suitable *jump conditions* to be satisfied across the *internal boundary* of the domain-partition. One result of the theory shows that for elliptic equations of order $2m$, with $m \geq 1$, the problem of establishing conditions for existence of solution for the *BVPJ* reduces to that of the *'standard boundary value problem'*, without jumps, which has been extensively studied. Background material of the "Theory of Partial Differential Equations on Discontinuous Piecewise-Defined Functions" appeared in scattered publications; however, the question of developing a *theory of partial differential equations in discontinuous piecewise-defined-functions* in a systematic manner was only recently addressed and published [41].

It should also be mentioned that a very important achievement of the theory just described, has recently been obtained in a paper that is in press [42]. Its relevance is in connection with the application of parallel computing to partial differential equations. The paper introduces a new approach to iterative substructuring methods that, without recourse to Lagrange multipliers, yields positive definite preconditioned formulations of the Neumann-Neumann and FETI types. Standard formulations are done using Lagrange multipliers to deal with discontinuous functions and this is the first time that such formulations have been made without resource to Lagrange multipliers. A numerical advantage that is concomitant to such multipliers-free formulations is the reduction of the degrees of freedom associated with the Lagrange multipliers. The general framework of the new approach is rather simple and stems directly from the discretization procedures that are applied; in it, the differential operators act on discontinuous piecewise-defined functions. Then, the Lagrange multipliers are not required because in such an environment the functions-discontinuities are not an anomaly that need to be corrected.

To finish, I hope that soon a new document, covering in a more complete manner MMC activities in Mexico, will be written. Then, I am sure, many other scholars whose work deserves attention will be included.

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Authors' CVs by Chapter

CHAPTER 1

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CHAPTER 2

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