Mathematics and Sciences

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Many mathematicians seem to agree that mathematics will enjoy a much healthier development in the new century if it is treated as an integral part of sciences. In the present article we will use this as a basic premise for discussing an important topic which concerns the part of mathematics that should naturally take up the task of bringing mathematics together with other areas of sciences – the applied mathematics.

One might argue that mathematics is more fundamental than sciences. After all it provides the language in terms of which scientific laws are stated. It provides the tools and techniques with which scientific calculations are carried out. It has its own set of questions as well as an intrinsic structure, the pursuit of which is driving much of mathematics today. There is no argument that a very impressive amount of mathematics was developed as a result of the quest for internal completeness, of studying the fundamentals such as numbers, equations and shapes. It is also true that as a fundamental part of our culture and knowledge, mathematics will always have its position as does philosophy, linguistics, and classics.

The issue is therefore not whether mathematics will survive but how to make it grow. In principle, mathematics should be in an advantageous position compared with other scientific disciplines for attracting talents, funding and public support. The intellectual ability of a child is often first revealed from his/her ability in mathematics. Most parents have a deep appreciation for the importance of their child's success in mathematics. Mathematics is a necessary background course for most science and engineering majors. It is heavily used in scientific research, industrial design and a host of other applications. However, over the years a gap has been created between mathematics education, application and mathematics research. While mathematics education/application is understood to be important by almost everyone, mathematics research remains largely a mystery to even the most educated public including our colleagues in other departments. There is a lot to be done before the mathematics community will be able to fully capitalize on the advantages mentioned above.

Computers have impacted our lives in a very fundamental way. They have changed the way that scientific and engineering research is carried out. Computation has become a major scientific tool in conducting research, playing comparable roles as does experiment and theory. When a new problem comes along, one of the first things to try is to find its mathematical formulation so that it can be modeled on the computer. Even though such a process of mathematicalization was also an essential part of scientific research in the old days, what happens now and what will happen in the future differs essentially from our past experience in at least two fundamental ways. The first is the time scale. It no longer takes years or decades to translate our understanding of nature into laws formulated in mathematical terms and have them checked quantitatively. The demand is that this process should happen in days or weeks. As a result, modeling and computation become a much more interactive process. The faster time scale also means that if mathematicians do not act quickly enough, they become irrelevant to such a process. The second is the form, variety and increased complexity of the problems. Mathematical models are no longer polished when they are presented to us. They are not necessarily clean. They may even be wrong! They certainly do not necessarily fall into the standard categories that we have set up for mathematical problems. This means that if we want to make an impact, we should be prepared to get our hands dirty.

Naturally the task of bridging mathematics with science and engineering falls on the hands of applied mathematicians, as it has been traditionally. Indeed applied mathematics has contributed greatly, in developing and analyzing the basic computational methods, in applications to fluid mechanics, structural mechanics and a host of other areas. Yet as the basic computational techniques become mature, more and more scientific disciplines are developing their own computational tools. Consequently computation as a whole is moving closer and closer to modeling. Can applied mathematics meet the new challenges and find and foster its new position in scientific research? Or will it adopt the current style of traditional pure mathematics and look into itself for future development? What are the new challenges in applied mathematics today? These are important questions that face all of us in mathematics, pure or applied. Below is a brief discussion of the author's view on some of these questions.

Research

Among the many interesting new directions in applied mathematics, we will discuss the following topics that we think will see most growth: first principle-based modeling, discrete models, stochastic effects and the combination of data analysis and modeling.

First principle-based approach to modeling. Much of the physical modeling relies on empirical laws based on physical intuition. It is astonishing that basic conservation laws plus the simplest linear constitutive relations describes so well the behavior of fluids at such a wide variety of situations, from creeping to turbulent flows, from water waves in a river to blood flows in a blood vessel. There is little need to refer to the underlying behavior of the molecules that make up the fluid. The same can be said for much of chemistry. The basic properties of chemical elements were found and the periodic table was discovered before its foundation was understood using quantum mechanics. The success of such empirical methods provided a strong push to extend them to more complex systems, with however mixed results. For example constructing empirical constitutive relations for polymeric liquids and plastic deformations prove to be a very difficult task. In many areas, scientists have now realized the limitations of the empirical approaches that bypass the microscopic details of the processes, and increasingly favor approaches that directly take into account the microscopics. Such a first-principle based approach is likely going to play bigger roles in the future for several reaons. One is that the improvement of computational power and computational methods will make it more feasible. The second reason is that the demand for more accuracy in our models, particularly for systems that fall in between scales described by well-established theories, such as nano-systems, will make it a necessity.

Examples of first-principle based approaches include the *ab initio* molecular dynamics [1] in which atomic forces are computed "on the fly" from the electronic structures, instead of using empirical potentials. Coupled hydrodynamic-kinetic models for polymeric fluids in which the extra polymeric stress is computed from the conformation of the polymers rather than empirical constitutive relations [4], the quasi-continuum method in which the stress and deformation of a material is found from atomistic interactions rather than empirical stored energy functional [5].

Discrete models. In applied mathematics, we are very used to modeling physical process using differential equations, i.e. the continuum models. While differential equations will continue to play a very pivotal role in applied mathematics, discrete models will certainly claim their role in the coming years. This is simply because many physical processes are naturally described by discrete models, such as discrete stochastic processes, molecular dynamics and kinetic Monte Carlo models. Examples are abundant in biology, ecology, materials sciences, and chemistry.

Discrete models bring out a host of new questions that should be addressed from the point of views that are quite foreign to us. Take the example of speeding up molecular dynamics. The traditional approach from the viewpoint of applied mathematics is to design ODE methods that allow large time steps or to process the models so that certain degrees of freedom that require small time steps can be eliminated. There is an alternative viewpoint, which is based on the observation that for many examples modeled by molecular dynamics, the system spends most of its time vibrating around local equilibrium states, with occasional sudden hops to different local equilibriums. The dynamics of the systems is characterized by these hopping events. It is therefore tempting to approximate the original molecular dynamics by a Markov chain that captures correctly the hopping events. This is the goal of the transition state theory [2] and has motivated a number of new techniques in speeding up molecular dynamics [3, 6].

Our interest in analyzing these discrete models will bring us closer to another important area of mathematics that has so far remained tangential to core applied mathematics, and that is mathematical physics. It is likely that mathematical physics will become a main ally for applied mathematics among the areas of pure mathematics, together with differential equations.

Stochastic effects. For historical reasons, stochastic analysis and stochastic methods have not become a standard tool for a large part of the applied mathematics community interested in scientific/engineering problems. Indeed when our main concern was fluid dynamics at intermediate scales or structural mechanics, there is little need to think about stochastic effects. However, things are different when we turn to material sciences, chemistry, biology and ecology. In these areas, stochastic effects are an intrinsic part of the problem. In some cases, they seem to have become the main obstacle for mathematicians to make further contributions.

Stochastic ideas also bring new tools into applied mathematics. A classical example is the Monte Carlo method for numerical integration. Other examples include the global optimization techniques and kinetic Monte Carlo methods. The performance of these methods is much less understood from the point of view of numerical analysis, and there is certainly a lot of room for important contributions.

We should note that discrete models and stochastic methods themselves are not foreign to applied mathematics. They play important roles in areas such as network models, finance, statistics, and control theory. One important direction of research will be to integrate the knowledge we have learned from these areas with applications to sciences.

Modeling and data analysis. Another interesting new direction of research is combining data analysis with modeling. In many applications, the underlying laws of nature are not known or not known at the scales of interest. It can also be that some of the important parameters are not known. In such cases, one might want to extract the governing laws or parameters from available data. One particularly attractive approach is to start the simulation with a complex, microscopic model and extract a simplified macroscopic model as computation goes on using the computed data. In other words, the numerical algorithm learns in the process of the computations. Such "learning algorithms" should combine scientific modeling with data processing techniques. These ideas already exist in various forms but they should be explored in much larger scale in computational sciences.

Education

At a time when applied mathematics should be aggressively moving into new areas of sciences, we also have to think carefully about how to train our students to best prepare them for the many different new challenges that they will face.

Students in applied mathematics should be cultivated both in mathematics and other sciences. They should receive a solid training in both the fundamentals of pure mathematics and the fundamentals of sciences. This should be our basic principle in education. This is undoubtedly a very difficult task. But perhaps it is not more difficult than the task Landau faced when he formulated the basic curriculum for theoretical physics, of which mathematics is an essential part.

Our current graduate curriculum is still very much in tune with "traditional" applied mathematics with strong emphasis on differential equations, continuum mechanics and numerical methods. Some applied mathematics graduate curriculum contains only these topics. While they will no doubt continue to play key roles in the future graduate curriculum, appropriate weights also have to be given to new emerging topics such as stochastic and statistical methods, and the basic principles of sciences. Some well-established courses, such as numerical methods, have to be modified in order to give more emphasis on areas such as molecular dynamics and Monte Carlo methods. For applied mathematics students interested in sciences and engineering, we propose a set of four courses as the basic core graduate curriculum. These are: computational methods, applied differential equations, applied stochastic methods, and introduction to scientific modeling.

Computational Methods. This is perhaps the most well-established course among the four proposed courses. However, current teachings of this course need to be modified in at least two aspects. 1. It needs to be streamlined, to be taught more efficiently, in order to make room for other new courses. 2. More emphasis has to be put on discrete simulations such as Monte Carlo methods and molecular dynamics, as well as computations based on quantum mechanics.

Applied Differential Equations. This course should cover rigorous analysis of prototypical equations, qualitative techniques such as bifurcation analysis and invariant manifolds, analytical techniques such as transform methods and asymptotic methods. It should also cover prototypical equations from applications such as fluid mechanics, nonlinear diffusion, material sciences, etc.

Applied Stochastic Methods. As we discussed earlier, stochastic analysis and stochastic methods will become a major tool in applied mathematics, along with numerical methods and differential equations. It is important to develop a course that is tailored to the needs of applied mathematics students interested in sciences. Such a course may contain the following list of topics: A quick introduction of random variables and limit theorems, Markov chains and Markov processes, stochastic differential equations, Fokker-Planck equations, path integrals, Monte Carlo methods, and rare events. A course that covers these topics is now developed at Princeton University and New York University.

Introduction to Scientific Modeling. It is difficult to decide on a best title for this course. We intentionally avoided calling it "Mathematical Modeling" since this course is intended to be a systematic introduction of the basic theoretical tools for modeling scientific problems. But we also have in mind to select those topics that are more mathematical, with a clear distinction between first-principle based methods and empirical methods. Much of these will be physics, since it provides most of the theoretical tools that are now used in every scientific discipline. But the teaching of it can be tailored to the needs of mathematicians.

Among the four courses discussed, this is perhaps the most difficult course to be developed and matured. The purpose of this course is to teach students basic principles, techniques and languages in sciences. Such a course is needed for several reasons. Our students may work in a variety of scientific disciplines and they may change their interest later on in their career, therefore a course limited to say, fluid mechanics, is not sufficient for the preparation of their scientific background. Currently students are encouraged to take such courses from individual departments outside of mathematics. While this will continue to be an important way that our students learn sciences, two factors have to be considered when we send our students to other departments. The first is that this is often time-consuming. Many topics covered in these courses are of little interest and/or importance to our students. If a student is interested in phase transformation in solids, he/she may not be able to afford the time to take one course in continuum mechanics, one course in statistical mechanics, one course in quantum mechanics or solid state physics. The other factor is that our students are often uncomfortable with the way courses are taught in other departments. They are unhappy about the lack of precision, the readiness to resort to empirical solutions rather than analysis of the detailed process. While complexity of the real system often do not leave us a second choice besides sweeping things under the rug, a more complete picture about the successful techniques should be presented to the students before they are asked to accept the ad hoc approaches. Moreover, science courses in other departments are often taught with an eye on minimizing mathematical complexity. This is one short-cut that our students do not always need.

There is a real opportunity for a course like the one discussed here. Whether we are interested in biology, chemistry or material sciences, some common background is always necessary. This includes basic classical mechanics, statistical mechanics, quantum mechanics, diffusion process, atomic and molecular structures, and continuum modeling. Concerning style, emphasis should be put on approximate analytical or numerical methods for solutions, on balance between deduction and rationalization, and on the relation between the microscopic and macroscopic processes.

Pure Mathematics. A remark is in order concerning the teaching of abstract mathematics to students in applied mathematics. This is an extremely important part of the education process. After all, mathematics is still our main tool and way of approaching problems. Abstract mathematics such as algebra, geometry, topology and functional analysis teaches us not only specific notions and techniques, but also the ability to extract a framework beyond the surface of concrete examples, to systematize concrete procedures, and to construct rigorous proofs. However our current approach to the teaching of abstract mathematics is rather unsatisfactory. Either it is mostly neglected or it is enforced through requirements in the graduate curriculum. In the latter case, students in applied mathematics are also required to pass exams in algebra, topology and/or geometry, etc. This often takes up the entire first year of their graduate school, leaving them less time for research, and most students fail to see the relevance afterwards. This has had rather disturbing consequences on the mathematical background of students in applied mathematics.

The point is that the teaching of abstract mathematics should also be streamlined. It is unrealistic to expect applied mathematics students to take separate courses in algebra, topology, geometry, etc., since they also need the time to study sciences and core applied mathematics courses. In most cases it is also unnecessary to go into that much detail in each of these subjects. Therefore it is highly desirable to design one course that introduces the basic notions, principles and techniques in abstract mathematics. The topics may include analysis on manifolds, group theory, Lie groups and Lie algebras, fundamental groups, intrinsic geometry, etc. This is also a good place for students to see the unity and beauty of mathematics, so results such as the Gauss-Bonnet theorem and Hopf theorem should be explained.

Academic Standards

Evaluating the work in applied mathematics can be a difficult, frustrating task. It is not surprising that opinions about particular pieces of contributions can be highly non-uniform. The main reason is quite simple. In applied mathematics, we are forced to use double standards: The mathematical standards and the scientific standards. Certainly rigorous proofs of existence of solutions to nonlinear systems of conservation laws should be considered an important contribution. But so is the fast Fourier transform, which does not use more than high school trigonometry, since it is so fundamental to computing. While mathematics has over the years developed a rather complete set of standards on the grounds of pure mathematics, most mathematicians including applied mathematicians are rather uncomfortable or unfamiliar with scientific standards. This is compounded by the fact that applied mathematics is continuously moving into new territories, leaving us little past experience that can be used to evaluate our work.

How do we resolve this situation? First and foremost, we should realize that while mathematics does and should have its own standards, ultimately our work will be judged by scientific and social standards. Secondly to be able to exercise scientific judgment, we as a community should become mature scientifically. We should educate ourselves. This is not just the task of applied mathematicians, but the task of the whole mathematics community. Realizing that there is more out there than the theorems we can prove and being able to adjust ourselves to that fact will ultimately lead the mathematics community to a new level of maturity.

At the same time, it is equally important for the applied mathematics community to become more cultivated in the basic values of core mathematics. After all, applied mathematics is still part of mathematics. It is different from engineering. Mathematical beauty, structure and techniques should be among its most important goals, and should also be used as a basic standard in evaluating its work.

Concluding Remarks

The maturing of the information age provides a great opportunity but also a great challenge to mathematics. Whether mathematics will grow or shrink depends on whether the mathematics community will be able to adapt to the needs of the applications. To deal with their own problems, the applied areas will use more and more heavily mathematics. Without the help from the mathematics community, they will develop the necessary mathematics on their own. This will lead to a separation of mathematics with the rest of sciences.

Applied mathematics should naturally take up the task of bridging mathematics with other scientific disciplines. To be able to meet such a challenge, we must attract the best talents to work in applied mathematics, to develop a solid curriculum, and to develop a balanced view of mathematics and sciences. Most importantly it should always be in touch with the frontiers of sciences. Nothing is more damaging to applied mathematics than isolating itself from the applications.

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References

[1] R. Car and M. Parrinello, " Unified approach for molecular dynamics and density-functional theory", *Physical Review Letters*, 55, 2471-2474 (1985).

[2] P. Hänggi, P. Talkuer and M. Borkovec, "Reaction-rate theory, fifty years after Kramers," *Rev. Modern Phys.* 62(2), 251 (1990).

[3] R. Phillips "Crystals, defects and microstructures", *Cambridge University Press*, 2001.

[4] J. Suen, Y. L. Joo and R. C. Armstrong, "Molecular orientation effects in viscoelasticity", *Annual Review of Fluid Mechanics*, 2002.

[5] E. B. Tadmor, M. Ortiz and R. Phillips, "Quasicontinuum analysis of defects in crystals," *Phil. Mag.*, A73 , 1529–1563 (1996).

[6] A. F. Voter, "Hyperdynamics: Accelerated molecular dynamics of infrequent events", *Physical Review Letters*, 78, 3908-3911 (1997).