

Development of a Sustainable India-United States program on Discrete Mathematical Modeling in Chemistry and allied sciences: A Conspectus of Two decades of Experience

By

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“No human inquiry can be a science unless it pursues its path through mathematical exposition and demonstration”

Leonardo da Vinci

“Those alone are wise who act after investigation.”

Charaka

“We haven’t got the money, so we’ve got to think.”

Ernest Rutherford

I. SOME PREFATORY REMARKS: RATIONALE AND GENESIS

Exercises on mathematization of chemistry have come to stay. Mathematical and computer modeling in chemistry, chemoinformatics, bioinformatics and allied sciences had a strong growth spurt in the second half of the twentieth century. This phenomenon was fueled primarily by two factors: 1) Novel applications of mathematical concepts, discrete mathematics in particular, to chemical and biological systems and 2) Availability of high speed computers and associated software whereby hypothesis driven as well as discovery oriented research could be carried out on a reasonable time frame. Fallouts of such research have led not only to obtaining new insights at the fundamental level, but also to significant applications in such critical areas as new drug discovery, protection of human as well as ecological health, chemoinformatics, bioinformatics, and computational biology, to name just a few.

Even before the advent of the twenty first century, Basak and Sinha felt the need of creating international and interdisciplinary forums to discuss the implications of developments mentioned above in basic and applied research as well as to sensitize young minds from around the world about the advancements in these areas. *They began discussions on the formulation of a regular binational India-United States Workshop/Conference series in the early 1990s and finally succeeded in organizing the first such event at a University, namely, Visva-Bharati University, India, in 1998.* This forms the genesis of Indo-US programmes on emerging areas and on a collaborative basis.

II. INDO-US WORKSHOP ON MATHEMATICAL CHEMISTRY

In 1998, with strong support from leading scientists and colleagues from around the globe, Subhash C. Basak (University of Minnesota, Duluth) and Dilip K. Sinha (then the Vice Chancellor of Visva Bharati University, Santiniketan, India) organized the first event of the Indo-US Workshop on Mathematical Chemistry series (<http://www.nrri.umn.edu/indousworkshop>). The objective of this series was to bring both senior scientists and young scholars to a single and homely forum in order to discuss the advancing frontiers of mathematical chemistry and allied sciences. The 1998 workshop was organized by Visva-Bharati University and University of Minnesota Duluth - Natural Resources Research Institute (UMD/ NRRI) with support from the Council of Scientific and Industrial Research (CSIR), India, and few other organizations at the all India level. This programme triggered off subsequently six more events of the series both in India and USA : the Second

Indo-US Workshop on mathematical chemistry at UMD, USA in 2000; the third workshop at UMD in 2003; the fourth workshop at the University of Pune, India, in 2005; fifth Indo-US Workshop was held UMD, USA, in 2008; the sixth event of the series was organized at the Heritage Institute of Technology, Kolkata, India, in 2010; and the seventh Indo-US Workshop was held at PRIST University, Thanjavur, India, in 2012. Throughout these years Subhash C. Basak and Dilip K. Sinha continued as the chairpersons of this binational workshop series from the United States and India, respectively.

It is worth mentioning that each of the seven Indo-US Workshops organized between 1998 and 2012 was enthusiastically attended by established scientists as well as young scholars from many countries of three to four continents. Consequently, *the seven successful events already organized have catapulted the Indo-US Workshop on Mathematical Chemistry series into a regular reference meeting of the scientific field worldwide*! The high quality of scientific discourse at the events of this series is evident from the fact that a large number of papers from the speakers have been published in the prestigious international journals like Journal of Chemical Information and Computer Sciences (JCICS), Journal of Chemical Information and Modeling (JCIM) after proper peer review. It is needless to mention that the training of young scholars and creation thereby of valuable human resources were important objectives of this initiative in line with the current nature of the global knowledge based economy. Some lead speakers were, for example, Professors Alexandru Balaban (Romania), Krishnan Balasubramanian (US), Danail Bonchev (Bulgaria) Rainer Bruggemann (Germany), Frank Burden (Australia), Jose Luis Villaveces Cardoso (Colombia), Jorge Galvez (Spain) Haruo Hosoya (Japan), Alan Katritzky (USA), Douglas Klein (USA), Paul Mezey (Canada), Marjana Novic (Slovenia), Milan Randic (USA), Roberto Todeschini (Italy), Nenad Trinajstić (Croatia), Nikolay Zefirov (Russia)who happen to be pioneers and outstanding contributor in mathematical and computational chemistry. The areas covered by them were both basic and applied aspects of mathematical chemistry and its applications in chemobioinformatics.

III. INDO-US LECTURE SERIES ON DISCRETE MATHEMATICAL CHEMISTRY

While the activities of the Indo-US Workshop series could move on uninterruptedly, it was felt that a separate forum was needed to bring the young scholars in close contact with the internationally renowned experts for exclusive mentorship and training. With this end in view, the Indo-US Lecture Series on Discrete Mathematical Chemistry (www.nrri.umn.edu/indouslecture) began in 2007 with the first event held at the PESIT College Bangalore sponsored by the Indo-US Science and Technology Forum, Department of Science and Technology (DST), Government of India, the International Society of Mathematical Chemistry (ISMC), and University of Minnesota Duluth/ Natural Resources Research Institute (NRRI), USA. For all events of this series, Subhash C. Basak has been the Chairperson from USA while various scientists from the Indian institutions acted as chairpersons depending on the host institutions in the country. The second event of the series was organized at Kalpetta, Kerala (supported by DST, UMD/ NRRI, and ISMC) in 2007; the third lecture series was held in 2008

sponsored and organized by Bharathidasan University, Tiruchirappalli, India, ISMC, and UMD/ NRRI; the fourth lecture series was organized in 2009 on the campus of Nizam College, Osmania University, Hyderabad, India, supported by the Indo-US Science and Technology Forum, ISMC, and UMD/ NRRI.

The courses and presentations of the Lecture Series were designed in such a way that it would target students of graduate courses (registered for PhD), post graduate courses, and in the final year of under-graduate courses of mathematics, physics, biophysics, chemistry, biochemistry, microbiology, bioinformatics, pharmaceutical chemistry, marine biology, etc.

In keeping with the spirit mentioned above, it was emphasized to the presenters/ lecturers that the lecture series should offer a forum for scientists so as to equip budding scientists in the various domains where discrete mathematics finds applications. The resource persons or lecturers, who were significant contributors in their respective fields, came from academia, regulatory agencies, industry, and government research institutions in USA, India, and other countries from Asia, Europe, and North America. The proceedings of the Lecture Series were made available to the attendees as reference materials. *The comments from the trainees indicated that they were highly satisfied with the intensive interaction they had with the speakers and others.*

IV. MATHEMATICAL CHEMISTRY WORKSHOP OF THE AMERICAS

Although the two sets of events mentioned above, Ind-US Workshop and Indo-US Lecture Series, appear from their titles to be nothing more than a couple of binational forums involving scientists from India and USA, in reality both of them were international academic platforms where scientists from countries outside USA and India routinely participated in large numbers. In fact, each of the events of the two series was regularly attended by senior scientists and young scholars from three to four continents. This led to a worldwide intellectual fermentation and stimulated collaborative research as well as spawning of other conferences, one example being the Mathematical Chemistry Workshop of the Americas

(<http://sites.google.com/site/mathchemamericas/>) involving countries of North and South Americas. Young scholars from South America were coming as participants in the Indo-US workshops and Indo-US lecture series both in USA and India with great interest. One such young participant, Dr. Guillermo Restrepo, and a senior mathematical/ computational chemist from Colombia, Professor Jose Luis Villaveces Cardoso, joined forces with Subhash C. Basak to initiate the Mathematical Chemistry Workshop of the Americas series in 2009. Basak, Restrepo (Universidad de Pamplona), and Villaveces Cardoso (UNIVERSIDAD DE LOS ANDES, Bogotá, Colombia) have been the chairpersons of the series from North America and South America, respectively. The first event of the series was organized at the UNIVERSIDAD DE LOS ANDES, Bogotá, Colombia, in 2009. Papers presented at this workshop were published in the peer-reviewed journal Current Computer Aided Drug Design

(<http://www.benthamscience.com/ccadd/EBM.htm>). The second event of the series was held both at the UNIVERSIDAD DE LOS ANDES, Bogotá, for four days and also at the University

of Pamplona, Pamplona, Colombia, for two days. Scientists and young scholars from four continents, viz., Asia, Europe, North America, and South America participated in the deliberation of the Second Mathematical Chemistry Workshop of the Americas with great enthusiasm. An electronic book (Ebook) is also being currently organized based on the presentations of these workshop held in Colombia.

V. THE WAY FORWARD

Looking back to the thirteen (13) mathematical chemistry events of the three series already held around the world, eleven Indo-US workshops/ lecture series and two workshops of the Americas, it is clear that discrete mathematical modeling is viewed by a wide range of scientific practitioners to have importance both for basic research as well as practical applications. The structure of objects of research in diverse disciplines, e.g., chemistry, physics, engineering, computer science, biology, chemoinformatics, bioinformatics, ecology, linguistics etc., can be represented by discrete mathematical models like graphs. Characterization and manipulations of such objects can give rise to fundamental understanding of the subject matter, e.g., molecular and submolecular basis of properties in chemistry and physics. Both linear (1,2,3) and nonlinear (4, 5) conceptualizations and applications can be utilized in model building and analysis. A recent trend in many branches of physical, environmental, and biomedical sciences is to understand systems in terms of networks. Discrete mathematical methods have come up with powerful tools in this area (6, 7, 8). Crisis and disaster management studies have, of late, brought to the fore the importance of risks and vulnerabilities in situations that are characterized by discrete elements (, 9, 10). The ongoing climate scenarios both in USA and India require a compelling investigation into discrete oriented conceptualization.

On the other hand, during the past few decades such methods have pervaded many practical disciplines like new drug discovery and hazard assessment of pollutants. To give an example, the discovery of one life saving drug currently costs more than one billion US dollars and takes more than ten years on the average. Of the three methods of screening chemicals for drug discovery—the low throughput *in vivo* testing, the medium throughput *in vitro* bioassays, and the high throughput *in silico* models—the last one based on mathematics, often discrete mathematical research and useful software derived thereby, is the least expensive and fastest of the three approaches. Intensive research on the basic aspects of such methods can lead to newly trained young scientists (manpower development), creation and marketing of new software (entrepreneurial activity and small business stimulation) leading to substantial enhancement of economic activities.

It is hoped that scientists, administrators, and policy makers of both USA and India recognize the importance of the Indo-US Series described here and come forward to take steps in order to consolidate the gains already realized by the limited resources of the organizers.

VI. CONCLUDING REMARKS

The foregoing lines provide broad glimpses of what could happen as opportunities provided by limited occasions of Indo-US interactivity, in the realms of widening areas of mathematical chemistry. A wider description shows a nuanced sequence of themes in the Conferences and even in lecture series. Any hindsight reveals a close analogy with sequels on programmes of the erstwhile National Council of Science Education and Research in collaboration with US counterparts. Hence, a totality of the above describes close kinship. The characterization of Indo-US relationship pertaining to science, science education, and research ought to find new dimensions through possible linkages. Thus, appropriately well-structured joint ventures may be envisaged so that innovative forms of characterization of such a relationship can flourish fruitfully. The Appendices here bear testimony to the sort of innovative framework that could be built up through the last two decades.

APPENDIX I

GUEST EDITORIAL

Fourth Indo-U.S. Workshop on Mathematical Chemistry, January 8-12, 2005, Pune, Maharashtra, India

“The Fourth Indo-U.S. Workshop on Mathematical Chemistry with applications in drug design, risk assessment of chemicals, chemoinformatics, bioinformatics, computational biology, and toxicology was held on January 8-12, 2005, in Pune, Maharashtra, India, under the joint sponsorship of the Natural Resources Research Institute (NRRI) of the University of Minnesota, Duluth, U. S. A., and the University of Pune. This issue of the Journal of Chemical Information and Modeling contains papers presented at the workshop. The concept of the Indo-U.S. workshop series was originally conceived by Subhash Basak, a senior scientist at NRRI, and received enthusiastic support from Dilip K. Sinha, a mathematician and educator from India. Together, Basak and Sinha have remained the chairpersons of the biennial, international Indo-U.S. Workshop series from the U. S. A. and India, respectively. The first event of the series was held in 1998 at Visva Bharati University, India, where Dilip Sinha was the vice chancellor at that time; the second and third workshops were organized by NRRI on the campus of the University of Minnesota, Duluth. The success of the Fourth Indo-U.S. Workshop, with the participation of over 125 participants from five continents, shows that the workshop series has established itself as one of the most important conferences in the field. The quality of the presented papers published in this volume after peer review demonstrates the high standard of scientific discourse taking place at the workshop.

*Discrete mathematical chemistry has made important advances in the past 25 years. This has been fueled primarily by two factors: (a) the formulation of new concepts and (b) easy access to high-speed computers. Methods developed in this field have found applications in pharmaceutical drug design and hazard assessment of environmental pollutants. Interestingly, discrete mathematical concepts, originally developed for the characterization of chemical systems, are being extended to deal with the explosion of data in “omics” science, namely, genomics, proteomics, and so forth. A few of the 17 papers from the Fourth Indo-U.S. Workshop presentations published in this issue of JCIM are outstanding examples of this expanding **chemo-bioinformatics continuum**.”*

By

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