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Tenth Annual Science Research Sessions 2021

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Message from the Vice Chancellor

Prof. A. Rameez

Vice Chancellor

South Eastern University of Sri Lanka

I am very much pleased to write this message on the occasion of the Tenth Annual Science Research Session 2021 of the Faculty of Applied Sciences, South Eastern University of Sri Lanka. This Science Research Session is one of the major annual events of the Faculty and has been organized successively for the tenth year in 2021. The theme of this year's research session is "*Data Driven Scientific Research for Sustainable Innovations*," which explicitly focuses on the data driven scientific research that can contribute to sustainable developments and innovations in the country. It is a common knowledge that the data driven scientific research is more effective and productive than the theory driven scientific research.

The South Eastern University of Sri Lanka promotes new research, creates new knowledge, and disseminates the knowledge through different platforms. As such, this annual session also plays an important role in the dissemination of knowledge. South Eastern University of Sri Lanka also promotes and encourages researchers and practitioners participating from across the country to benefit from this research session in sharing their valuable research findings among well attended scholars and researchers. The ASRS-2021 provides a platform for researchers, academics and students from all over the country to interact and engage in academic discourses among themselves while presenting their research findings.

Lastly, I would like to take this opportunity to congratulate the chair, coordinator, secretary and the organizing committee of the Annual Science Research Session 2021 of the Faculty of Applied Sciences, SEUSL for their tireless effort and commitment in organizing the event virtually in the present context of the COVID-19 pandemic. I also wish to thank all others who have contributed to make the research session a reality. Finally, I wish the Tenth Annual Science Research Session 2021 of the Faculty of Applied Sciences, South Eastern University of Sri Lanka a great success.

Message from the Dean

Dr. U. L. Zainudeen

Dean

Faculty of Applied Sciences

Faculty of Applied Sciences is proudly hosting the Tenth Annual Science Research Session 2021 (ASRS-2021). This research conference is one of the prime events organized annually by the faculty and theme of ASRS-2021 is *"Data Driven Scientific Research for Sustainable Innovations"* which is an appropriate and timely theme for present global trend. This Conference aims to bring leading and young researchers involved in all branch of science together so that they will have a forum to share their experiences, research outcomes and creativity and innovative ideas in science and its contemporary applications.

Our Faculty of Applied Sciences offers many courses through its five departments namely Biological Sciences, Physical Sciences, Chemical Sciences, Mathematical Sciences and Computer Science. In addition to the Bachelor's programs, the faculty offers Postgraduate Diploma programs, Master of Philosophy and Doctor of Philosophy degree programs as well. The faculty also involves in carrying out innovative research and development. Despite of the challenges the faculty faced due to the ongoing COVID-19 pandemic; the faculty is being progressing successfully with its schedule. Total credits go to all members of the faculty and students. In this line, the faculty organized the conference in virtual mode with support of the technical committee.

I wish to thank all members of the organizing committee of the 10th ASRS-2021for their tremendous supports and hard work to make the conference successful. I extend my sincere gratitude to Dr. M.C. Alibuhtto, conference coordinator and Dr. (Mrs) P. V. H. K. Ranasinghe, conference secretary for their dedication and amazing contributions.

I wish the conference very successful.

Message from the Coordinator

Dr. M. C. Alibuhtto

Coordinator/ASRS-2021

It is with great pleasure, I convey this message to the proceedings of the 10th Annual Science Research Session (ASRS) -2021, Faculty of Applied Sciences, South Eastern University of Sri Lanka organized under the theme *"Data-Driven Scientific Research for Sustainable Innovations"*. The annual science research session focuses on dissemination of research problems, solutions, and insights on new challenges faced in the field of modern sciences. Fifty-six extended abstracts in various subjects were received from researchers and reviewed by eminent reviewers, out of these 34 were accepted for presentation and 10 for publication in our JSC communication journal. The event will be delighted by a keynote speech and a guest speech by two eminent professors followed by nine parallel technical sessions consisting of 44 oral presentations.

I would like to convey my deep gratitude to Prof. A. Rameez, Vice Chancellor and Dr. U.L. Zainudeen, Dean, Faculty of Applied Sciences for their guidance and fullest support in organizing this important event. I also express my sincere thanks to the keynote speaker, Professor Rohan Samarajiva, the Chairman, LIRNEasia and guest speaker Assistant Professor W. M. C. Sameera, Hokkaido University of Japan.

I would like to extend my heartfelt appreciation to all the members of the academic staff, the administrative staff and the non-academic staff of our faculty. Further, my sincere thanks to all authors and presenters at the tenth ASRS who are the major contributors to this event. Also, I take this opportunity to thank the secretary, members of the editorial committee, reviewers, organizing committee, sub-committees, and all the panellists for their valuable contribution in various ways to make ASRS-2021 all success.

I wish all the participants a wonderful experience at the conference.

Acknowledgments

Dr. Kokila Ranasinghe

Secretary/ASRS-2021

"We must not forget that when radium was discovered no one knew that it would prove useful in hospitals. The work was one of pure science. And this is a proof that scientific work must not be considered from the point of view of the direct usefulness of it. It must be done for itself, for the beauty of science, and then there is always the chance that a scientific discovery may become like the radium a benefit for humanity"

– Marie Curie, during a lecture at Vassar College, Poughkeepsie, New York (14 May 1921)

It gives me immense pleasure to pen this acknowledgement note, as the Faculty of Applied Sciences, SEUSL holds the tenth Annual Science Research Session (ASRS-2021). The ASRS is one of the main events organized by FAS, where the faculty showcases its research potential and networks with researchers coming from all over the island.

On behalf of the FAS and the University, I am grateful to Prof. Rohan Samarajiva for agreeing to serve as the keynote speaker, and to Dr. W. M. C. Sameera for sharing his cutting-edge research expertise with us. I profusely thank our vice chancellor, Professor A. Rameez, for gracing our occasion as the chief guest. A special note of thanks goes out to the dean of FAS, Dr. U. L. Zainudeen, for his mentorship throughout the process of organizing this event. I appreciate and sincerely thank the members of the organizing committee and the editorial board of ASRS-2021 for their untiring commitment to make this a memorable event. Further, the support extended by academics, administrators, and support staff of FAS is deeply appreciated and the contribution made by our own students in various aspects including graphics and art work is highly commendable. My heartfelt gratitude goes to the reputable article reviewers for their service. Last but not least, I thank all the researchers who chose ASRS-2021 to present and discuss their hard-earned research successes. I hope that the dedication and teamwork we accorded during the past few months will lead to a remarkable symposium!

Keynote Speaker: Biography and Essence of Keynote Speech

Prof. Rohan Samarajiva

Chair

LIRNEasia, Colombo, Sri Lanka

Rohan Samarajiva is founding Chair of LIRNEasia, an ICT policy and regulation think tank active across emerging Asia. He was CEO for eight years from its inception in 2004. His most recent co-authored book (2013) is Information lives of the poor: Fighting poverty with technology, published in Burmese, English, French and Spanish. He is a member of the UN Global Pulse Advisory Group on the Governance of Data and Artificial Intelligence. He served on its predecessor, the Data Privacy Advisory Group, since 2015. Samarajiva currently serves on the Specialty Board in Biomedical Informatics and as Examiner, MSc in Biomedical Informatics & MD in Health Informatics, Postgraduate Institute of Medicine, University of Colombo. He served as Chair of the ICT Agency, the apex body for information and communication technology within the government of Sri Lanka, in 2018-19. He was one of its founding directors in 2003-05.

He was Team Leader at the Sri Lanka Ministry for Economic Reform, Science and Technology (2002-04) responsible for infrastructure reforms, including participation in the design of the USD 83 million e Sri Lanka Initiative. Samarajiva was Director General of Telecommunications in Sri Lanka (1998-99), Honorary Professor at the University of Moratuwa in Sri Lanka (2003-04), Visiting Professor of Economics of Infrastructures at the Delft University of Technology in the Netherlands (2000-03) and Associate Professor of Communication and Public Policy at the Ohio State University in the US (1987-2000).

Data science research in Sri Lanka: Human resource challenges and prospects

Based on the experience of building a data analytics unit within a Sri Lankan research organization since 2012, this presentation examines the challenges of doing cutting-edge data science in Sri Lankan conditions. Open-source software and relatively inexpensive hardware have lowered the barriers to participation. Constraints such as problems of access to data sets and funding are discussed briefly, with emphasis being placed on the challenges of recruiting and developing research personnel with the required skills. The field is subject to rapid change, with the even terms such as big data, now being replaced by newer terms. The importance of continued learning and working in interdisciplinary teams is highlighted.

I was fortunate to have the opportunity to serve on the faculty of the Ohio State University, one of the largest state universities in the US, from 1987 to 2000. This was an exciting time. Search engines were beginning to transform the entire web experience. What had been once an esoteric insiders' club of academics and researchers was being made into the global public space it is today. The socio-political and economic aspects of the Internet and the massive rise in data communication was beginning to attract the attention of researchers. I attended the first Computers, Freedom, and Privacy Conference, and owned a copy of the first Wired magazine.

We understood from the start that the study of the socio-political and economic aspects of the emerging technologies had to be inter disciplinary. As the recipient of a grant to get this conversation going, I found myself talking to senior professors at the Ohio Super Computing Centre, in university's own Computing Centre, in the Engineering Faculty, in the School of Public Policy and so on. One of the curious things I noticed was how many of these pioneers had PhDs in Chemistry. I asked around as to why.

The answer was staring me in the face. In the early days of computing, there were no computer science PhDs; there were no computer science BScs; there were no computer science departments. By necessity, everyone who was a pioneer in computing applications was a graduate in some other subject. At Ohio State, the scientists in the Department of Chemistry were writing computer programs for their research and had obtained the required hardware through the grants they obtained. They then rose in the various computer-related centres that they built up, and some of them gave up on chemistry. In other places, physicists may have taken on this role; at Ohio State it was chemists.

These memories from the 1980s became relevant when I and Sriganesh Lokanathan, now Data Innovation and Policy Lead at Pulse Lab Jakarta (a joint venture of the UN and the government of Indonesia), ventured into research on big data applications and policy in 2012, almost 10 years ago. They are relevant today as well because researchers with the required skills and attitudes are the most significant constraint.

Big data research. Back in the 1990s, I was working on what we now call "big data," but there were few at the university who could conduct research using these massive data sets. One needed access to super computers made by companies like Cray. These machines were so expensive and significant that the business pages reported individual sales; the number of countries that owned them could be counted on two hands. My research was on the policy implications of these novel capabilities made possible by these super-fast processors capable of handling massive data sets.[1] When I came to Sri Lanka to work on telecom sector reforms, I closed off that line of research and focused on research relevant to our conditions.

In around 2009, reports of a new kind of data-based research appeared. An example was Google's efforts to track the emergence of seasonal flu outbreaks in the US by analysing the terms used in billions of searches across the country. The claim was that the seasonal variations in search terms could tell decision makers which areas were experiencing flu outbreaks. Even though it was not a representative sample of the population, it was claimed that it was highly accurate.[2]

I wondered what kind of computing power they were using for that kind of near real-time analysis. But the pieces came together only in 2011 when I was listening to IBM Fellow C. Mohan speak in Colombo at an event organized by WSO2, a leading software company. I learned that supercomputers were no longer needed to analyze massive data sets, that major advances in storage memory allowed researchers significantly higher flexibility, and that the software was open source. We quickly put together a proposal to raise fund to conduct big data research of relevance to urban planning, a hot topic in the post-war conditions of 2011. I managed to negotiate access to pseudonymized mobile network data from multiple operators.[3]

The funders in Canada were very positive about the opening up of a new research front, but they had one question: did we have the people to do the research? It was a simple but decisive question. The funding decision rested on an adequate answer being provided.

Luckily, we had done some big-data-like research with a grant from the same funding agency a few years earlier. This was a collaboration with a lab at Carnegie-Mellon University in the US where we were trying to identify emerging diseases and propagation of infectious diseases.[4]

It was different from what we describe as big data research in two aspects. One was that we were creating the data for analysis by positioning assistants next to doctors as they examined patients. This is very cumbersome and cannot be sustained over time (the project gave good results but died as a result).

The second difference was that we were not doing the analysis ourselves. The lab at Carnegie Mellon had developed T-Cube, something they then described as "learning software" to analyze and predict faults in US Air Force aircraft. They wanted to see what other tricks could be taught to the software. Our data, with all the personally identifiable elements stripped out was run through T Cube and would spit out analyses of various patterns. In today's terms this was a machine learning application, that some would even describe as Artificial Intelligence. But it was still in that old paradigm: expensive super computers and proprietary software.

But the principal investigator on the project that used T Cube was Nuwan Waidyanatha, a brilliant US trained mathematician with a Masters in Operations Research. He was no longer working fulltime for us, having moved to Kunming, China, but we could claim that he would be part of the team. The other key person was Sriganesh Lokanathan, who had a Computer Science first degree from MIT and a master's in public policy from the Lee Kuan Yew School at the National University of Singapore. They would do the analytical work, while I would supply the policy expertise and serve as data wrangler. The funders accepted our response that we had a core team in place. The grant was approved.

Challenges. Once we obtained the funding, we found that Waidyanatha could not actually play a role, for various reasons, including location in China. The data were bound by strong non-disclosure agreements (NDAs) and could not be used outside our office. Lokanathan had the foundational knowledge in computing, but the languages and techniques used for analysis of big data in 2012 were not known when he was at MIT. This meant that he was scrambling to find people to conduct the research while rapidly educating himself on the required skills.

Continuous learning

We got lucky. Our first part-time researcher was Nisansa de Silva, a computer science graduate from Moratuwa, who was both a hard worker and a fast learner. Through him, we were able to recruit a core team of University of Moratuwa graduates who wanted to do cutting-edge research and get the publications that would enable them to enter good post-graduate programs. Now they all have PhDs or all about to get them. Dr de Silva is back as a Lecturer at the University of Moratuwa. This first set had a solid foundation in computer science, but had to learn data analytics while working. We also established working relationships with Joshua Blumenstock, perhaps the leading researcher using big data to generate development-related insights, and with colleagues from the MIT economics program.

Beyond the initial team we recruited many interesting researchers with varied backgrounds. Aparna Surendra is illustrative. When she came to us wanting to work as an intern, having no formal qualifications in computing; she was an English Major with work experience in international relations. But she was already taking online courses in data science and was from Stanford, where

the very air people breathe seems to include computing. She did excellent work with us,[5] went on to get a placement as an intern at Deep Mind, one of the world's most prestigious artificial intelligence companies, and is now Senior Associate at AWO Agency, a leading data rights organization that blends data science, law and ethics.

Big data was the focus of work back in 2012. But now the field has moved on. Everyone is working on what is colloquially known as artificial intelligence. That means that whatever our current researchers learned while at university is not enough. In the time sheets that all researchers complete so that their time can be billed to various projects, we introduced a column for time spent on learning. Everyone at LIRNEasia is expected to engage in learning; we not only allow paid time to be used for learning but in some cases, we will pay for the courses. We found that the researchers in the team that started off as big data (now called Data Algorithms and Policy) spent 25 percent of their time learning, double what other researchers did.

What this means is that the content of what was learned in degree programs prior to joining us matters less than the willingness and the ability to learn. Some knowledge of computing does help, as we have seen from some of our failure cases. But even the fully self-taught, like Aparna, can achieve excellent results. It appears that things are not much different from what was happening at Ohio State back in the 1970s, with people from various disciplines were boot-strapping themselves into computer scientists.

Interdisciplinary teams. Most, if not all, data science papers have multiple authors.[6] What we found was that the data science people had to know how to speak the language of the domain experts in whatever field they were working in. For example, our own work on dengue propagation,[7] included medical researchers; a paper on transportation included a transportation specialist.[8]

This is never easy, but possibly the US and Canadian university practice of requiring undergraduates to take courses outside their specialization provides an advantage to those who come from such systems as against the rigidly disciplinary curricula found in Sri Lanka. But it may be possible for newer programs to build in more opportunities for inter-disciplinary learning.

Our most successful data scientists have been those who were able to think beyond disciplinary boxes and read widely. I recall mentioning a book club organized outside office hours in my recommendation letters for one of our researchers who is completing a PhD in computational social science in the US.

Recruitment never stops. It is well known that data scientists are in short supply and that they are paid well. Even when the salaries are high, it is difficult to hold on to them. The strategy at LIRNEasia was to think of the compensation in terms of a package that included the opportunity to do innovative work and publish leading to higher probability of gaining funded admission to high-profile PhD programs. It is thus normal for researchers to cycle through.

This requires continuous recruitment and mentoring. For effective recruitment and mentoring it is necessary for there to be a stable core leadership team. When that condition cannot be maintained, the entire operation is weakened.

Funding. Research requires adequate levels of funding. Sri Lankan universities are limited in what they can pay researchers who work on funded projects. In addition, funding from outside the country now requires Cabinet approval, which is said to take inordinate time, given the layers of prior approvals required. These problems are likely to seriously disadvantage university-based data science research.

Access to large datasets. One must have big data in order to do big data research. This is especially important in the context of the heightened importance of machine learning. Obtaining access to datasets that are under the control of government agencies is difficult because of attitudes which are hostile to sharing and also because the quality of the datasets is problematic. For example, see the transport data on the government's open data portal,[9] where the most recent data is nine years old.

LIRNEasia did manage to gain access to valuable pseudonymized datasets from the private sector. The difficulties experienced are described in detail elsewhere.[10] With apparent adoption of the rather rigid European model of data protection,[11] it may become even more difficult for outside researchers to gain access.

If all data use has to be covered by consent and purpose limitation principles, it may not be possible to permit use by third parties for traffic management, energy management, urban planning etc., since these uses could not be conceptualized at the time of signing up customers. So, what is likely to be the result of mechanical extension of inform and consent rules that were developed for qualitatively different conditions of the past would be giving the big companies such as mobile operators or search providers a monopoly on large datasets of transactions; and shutting out small firms and social interest users.[12] However, there may be other datasets such as satellite data that are either public, or available for purchase, that can be used for research.

Prospects. The heyday of data science is actually behind us. For most purposes, what used to be done under the rubric of data science is now being done as AI research. In addition, completely new strands of research are being opened up such as Web 3.0.[13] It is unlikely that there will ever be a situation where what is taught in universities can be directly applied in cutting-edge research in any of these areas.

Universities will have to establish good working relations with research organizations and firms so that their students can learn what is happening at the cutting edge, while equipping them with foundational knowledge which is what universities are good at. In that sense, the story told above of a particular experience of setting up a big data research unit in Sri Lanka has broad relevance.

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Guest Speaker: Biography and Essence of Keynote Speech

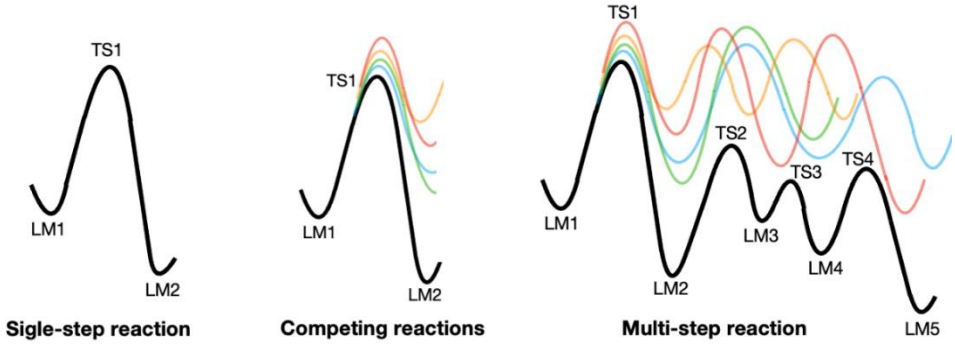
Dr. W. M. C. Sameera

Institute of Low Temperature Science, Hokkaido University, Japan

W. M. C. Sameera was awarded a B.Sc. (Hons) from the University of Sri Jayewardenepura and a PhD from the University of Glasgow in the United Kingdom. He was a postdoctoral researcher at Oxford University and the Institute of Chemical Research of Catalonia. Then, Sameera was a Marie Curie ITN experienced researcher at Gothenburg University in Sweden and a Japan Society for the Promotion of Science research fellow at the Fukui Institute for Fundamental Chemistry in Japan. In 2016, Sameera became an assistant professor at Hokkaido University in Japan. His research interest focuses on quantum chemistry and computational materials science. Sameera's research program is funded by the Japan Society for the Promotion of Science and Ministry of Education, Culture, Sports, Science and Technology in Japan. His research projects involve close collaborations with experimental research groups in Japan, Europe and the USA.

Quantum chemical modelling of chemical reactions

Atomic-scale modelling of chemical reactions is an important area of modern computational chemistry. The mechanism of a chemical reaction gives a detailed description of the atomic-scale processes, and such information is essential for experimentalists to design novel chemical reactions to synthesize chemicals, pharmaceuticals, and materials. However, the quantitative details of the reaction mechanisms are challenging to characterize in full from experimental methods. In this direction, computational chemistry has been made significant contributions. I develop computational methods to study mechanisms of the chemical reactions, employing quantum mechanics or quantum mechanics/molecular mechanics methods.[1-3]



The primary objective of a mechanistic study is to calculate the stationary points on the potential energy surface of the chemical reactions, in particular local minima (LMs) or transition states (TSs). Using the relative energy of the LMs and TSs, the reaction barrier can be calculated, and the reaction rate can be determined. If the reaction involves competing reactions, the selectivity of the reaction is essential. Some chemical reactions involve multi-steps. In such cases, the main goal is to calculate various possible reaction paths connecting the reactant and the product. After calculating the reaction barriers of the individual step of each reaction path, the lowest energy path can be determined, which is the mechanism of the reaction.

In my presentation, I will discuss puzzling reaction mechanisms relevant to catalysis and materials science.[4-8] With the novel computational methods in hand, now we can rationalize quantitative mechanistic details of the chemical reactions. Thus, computational chemists can guide experimental researchers to develop novel chemical reactions for potential applications in industry and academia.

References

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