





National Seminar on Computational Science and

Prof Sridhar R Gadre's 75th Birthday Festschrift Symposium

9 - 10 June, 2025

Somaiya Vidyavihar University, Vidyavihar, Mumbai



Organised By

Centre for Excellence in Computational Science and Simulations, Somaiya Vidyavihar University, Vidyavihar, Mumbai

In collaboration with

Srinivasa Ramanujan Institute for Basic Sciences (SRIBS), Kottayam

Somaiya Vidyavihar University

Established in 2019, Somaiya Vidyavihar University, Mumbai, is a self-financed university, recognised by the University Grants Commission (UGC) and sponsored by Somaiya Vidyavihar. Somaiya Vidyavihar University is a place where you can explore new possibilities, pursue your passion and find yourself.

Centre of Excellence in Computational Science and Simulations (C2S2)

Centre of Excellence in Computational Sciences and Simulations (C2S2) was inaugurated by Hon'ble Chancellor Mr Samir Somaiya, in presence of Hon'ble Vice Chancellor Prof V N Rajasekharan Pillai, and Prof S Sivaram (Professor of Eminence, SVU) on July 07, 2024.

The vision statement for C2S2: To explore the limitless possibilities of scientific computing, modelling, and simulations through innovation in education and research.

C2S2 will enhance the culture of teaching and research with a view "exploring science without boundaries". It is expected that the students will learn the essential concepts and the associated theories in the classroom and will get hands-on training with tools of computational sciences and simulations, early in their education. It's prime focus will be on offering interdisciplinary teaching programs, exploring independent research projects, outreach programs related to diversified domains of computational science and simulations, as well as enables the students to use the latest technology to perform effectively and efficiently.

Srinivasa Ramanujan Institute for Basic Sciences (SRIBS)

The Srinivasa Ramanujan Institute for Basic Sciences (SRIBS), a constituent of the Kerala State Council for Science, Technology and Environment (KSCSTE), fosters fundamental research across disciplines including chemistry, biology, physics, mathematics, and computer science. Established in 2012, SRIBS was inaugurated in 2013, and commenced operations at its Kottayam office on 9th Feb. 2014.

SRIBS stands as a testament to the Government of Kerala's commitment to fostering a vibrant research ecosystem in the state. Born from a vision to advance fundamental research in computational and theoretical sciences, SRIBS has steadily grown into a promising hub for scientific exploration and knowledge dissemination. With its state-of-the-art infrastructure, dedicated leadership, and commitment to scientific excellence, SRIBS is set to make significant contributions to knowledge creation, technological innovation, and societal progress. SRIBS aims to foster an environment where ground breaking research can thrive, promoting global collaborations and nurturing the next generation of Indian scientists.

National Seminar on Computational Science and Prof Sridhar R Gadre's 75th Birthday Festschrift Symposium

The field of computational science has transformed the way we approach problem-solving in various scientific disciplines.

Seminar Themes:

- · Method and algorithm development
- · Artificial intelligence and Machine learning applications
- Computational Chemistry and Physics
- · Computational Biology, Bioinformatics
- Drug discovery
- · Materials science
- Professor Sridhar R Gadre 75th Birthday Festschrift Symposium
- Special Feature: Poster Session for young researchers

Who should attend:

The seminar is aimed at introducing the

- UG/ PG Students
- Research Scholars
- Faculty Members and Scientists from R&D Institutes
- · Industry Delegates

To the current scenario of computational science, especially the state-of-the-art methods and algorithms along with the advanced topics from computational physics, chemistry, biology, and materials science. Furthermore, the seminar will feature a poster session to showcase and encourage the research work done by the young researchers and opportunity to interact with the experts.

Registration:

All participants of the conference must register for the conference.

Important Dates:

Abstract Submission

May 29, 2025

Abstract Acceptance May 31, 2025

Click to register

https://forms.gle/pnnF14caFGZwUyrR9

Registration Fee:

Research Scholars

UG/ PG Students : Free

: 2000/- INR

Faculty Members and : 4000/- INR

Scientists from R&D Institutes

:5000/- INR

Industry Delegates

Contact: Dr Anant D Kulkarni: anant.Kulkarni@somaiya.edu

Speakers:

- · Prof Shridhar R Gadre (SPPU, Pune)
- Dr Ajay C Limaye (Australian National University)
- Prof N Sathyamurthy (IISER, Mohali)
- Prof Upendra Natrajan (IIT Madras, Chennai)
- Dr C H Suresh (SRIB, Kottayam)
- Prof Sudip Roy (Prescience Insilico, Bangalore)
- Prof Prakash Zha (Central University, Gujarat)
- Prof Arun Venkatnathan (IISER, Pune)

- Prof A Anoop (Digital University, Kerala)
- Dr U Lourdraj (NISER, Bhubaneshwar)
- · Dr Ambar Jain (IIT, Mumbai)
- Prof Ateeque Malani (IIT, Mumbai)
- Dr P Balanarayan (IISER, Mohali)
- Dr Milind M Deshmukh (University of Delhi)
- Dr K V Jovan Jose (University of Hyderabad)

Patrons:

- Mr Samir Somaiya, Chancellor, Somaiya Vidyavihar University, Mumbai
- Prof V N R Pillai, Vice Chancellor, Somaiya Vidyavihar University, Mumbai
- Prof S Sivaram, Professor of Eminence, Administrative and Academic head, C2S2,
 Somaiya Vidyavihar University, Mumbai, Honorary Professor and INSA Senior Scientist, IISER, Pune
- Prof Neetin Desai, Dean, Faculty of Science, Somaiya Vidyavihar University, Mumbai
- Prof Santosh Narayankhedkar, Dean Academics, Somaiya Vidyavihar University, Mumbai

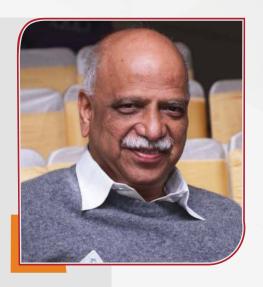
National Advisory Committee:

- Dr Sudhir A Kulkarni (NovaLead Pharma Pvt Ltd, Pune, Conference Chair)
- Prof S Sivaram (SVU, and IISER, Pune)
- Prof Swapan K Ghosh (University of Mumbai, Mumbai)
- Prof G P Das (TCG Centres for Research and Education in Science and Technology, Kolkata)
- Dr C H Suresh (Srinivasa Ramanujan Institute for Basic Sciences (SRIBS), Kottayam)
- Prof Rajeeva Karandikar (Chennai Mathematical Institute, Chennai)
- Prof Sathyamurthy (IISER, Mohali)
- Prof K L Sabastian (Indian Institute of Science, Bengaluru)

Local Organizing committee:

- Dr Anant D Kulkarni (Convener)
- Dr Daly Davis
- · Dr Suren Patwardhan
- Dr C V Avadhani
- · Prof Soumyadeb Ghosh
- Dr Sudip Roy

- Dr Deepti Gupta
- Dr Sagar A Marathe
- · Dr Vandana Jamdar
- · Dr Nilesh Wagh
- Dr Vaijayanti Ghase



Prof Shridhar R Gadre is one of the founding figures of Computational and Quantum Chemistry in India.

Prof Gadre is a Honorary Distinguished Professor, and INSA Senior Scientist at Departments of Chemistry and Scientific Computing, Modelling & Simulation, Savitribai Phule Pune University.

Research interests:

- · Theoretical and Computational Quantum Chemistry.
- Molecular electrostatics potentials and momentum densities.
- Chemical reactivity and weak interactions.
- Pioneered a technique called the Molecular Tailoring Approach.

Academic and Scientific Contribution:

- Founder and Director of Inter Disciplinary School of Scientific Computing (195), S P Pune University, Pune.
- Growth of computational technologies in Chemistry, Physics and scientific computing in India.
- Authored 247 scientific research articles published peer-reviewed core journals of very high international repute such as Chem Rev, J Amer Chem Soc, J Chem Phys, J Phys Chem, Phys Rev A, Chem PhysLett etc. as well as some invited contributions to edited books.
- Co-authored a book "Electrostatics of Atoms and Molecules".
- Mentored 18 PhD students and 46 Master's degree students.

Awards and Honors:

Received several National and International awards/ honors for his contribution to the field of computational and quantum chemistry that are:

- Elected as a Fellow of the Indian Academy of Sciences, Bangalore (1991).
- Fellow of the Indian National Science Academy, New Delhi (1996).
- Awarded the Shanti Swarup Bhatnagar Prize in Chemical Sciences (1993).
- J C Bose National Fellowship by the DST, New Delhi (2007).
- A mini-conference on Molecular Electrostatic Potentials was organized at Vrije University, Brussels, to honor his work in this area (2014).
- Awarded the Lifetime Achievement Award by the Indian Chemical Society (2022).

About Somaiya Symposium Series:

The Somaiya Vidyavihar University is committed to fostering a vibrant academic and research environment through the continuous organization of seminars and conferences. The earlier seminars/ Conferences/ Symposia were:

- 1. National Webinar on Recent Trends in Computational Chemistry (Aug. 2021).
- 2. National seminar on Polymer Science and Technology: Academia and Industry Perspectives (May 2022).
- 3. National Conference/Discussion Meeting on Simulations in Polymers, Materials and Biomolecules (June 2023).
- 4. Seminar on Computational Modelling and Simulations (July 2024).
- 5. Somaiya Polymer Science Symposia Series S4P 4th Edition (October 2024).

This Seminar is the 6th in the series which is SVU's ongoing efforts to organise seminars reflect its dedication to academic excellence and the continuous development of its students through collaborative learning and discussion.



The Somaiya Vidyavihar campus showing existing and proposed buildings of Somaiya Vidyavihar University and Somaiya Vidyavihar Institutions.