



Centre for Intelligent Solutions



About IISER Pune

The Indian Institute of Science Education and Research (IISER) Pune is a premier institute dedicated to research and teaching in the basic sciences. It was established in 2006 by the Ministry of Human Resource Development (renamed Ministry of Education in August 2020). In 2012, IISER Pune was declared as an Institute of National Importance by an Act of Parliament.

As a unique initiative in science education in India, IISER aims to be a Science University of the highest calibre devoted to both teaching and research in a totally integrated manner, with state-of-the-art research and high quality education, nurturing both curiosity and creativity.

At IISER Pune, we dedicate ourselves to learn, teach and serve society through excellence in education, research and public service, to create a learning and working environment based on integrity, fairness, dignity and professionalism, to provide equal opportunities for all, and to develop and encourage a sense of environmental responsibility.

Research at IISER Pune is carried out at the departments of Biology, Chemistry, Data Science, Earth and Climate Science, Humanities and Social Sciences, Mathematics, Physics and Science Education. Interdisciplinary research at the interface of one or more disciplines are also being actively pursued. It maintains a vibrant research atmosphere fuelled by the faculty and the students. As a premier academic and research institution, the research facilities at IISER Pune is one of the best available in the country. IISER Pune also attracts a wide spectrum of experts from within and outside India for academic programmes and other events such as conferences and workshops held in the campus throughout the year.

Centre for Intelligent Solutions

At the core of the fourth industrial revolution, or Industry-4.0, is the digital transformation characterised by an enhanced use of data, analytics, and connectivity in all industrial processes from manufacturing to services. The emerging tools of artificial intelligence and data sciences carry a promise for disruptive changes in all of these areas. In contrast, quantum technologies promise exceptional computational speed and efficiency for certain niche problems. These anticipated changes are powered as much by data availability as by faster algorithms, novel mathematical frameworks, computational tools, and digital transformations.



The Centre for Intelligent Solutions at IISER Pune addresses industry-focussed problems lying broadly within the markers of data, algorithms, models, applied mathematics, computation/simulation, and digital transformations. The Centre brings together more than twenty researchers of IISER Pune and aims to promote technological innovation led by researchers of IISER Pune working on various computational and mathematical sciences.

For the industry, this Centre provides opportunities for engaging in joint research projects, consultancy, student projects, placements, and many others with IISER Pune. In the years to come, this Centre is expected to play a leading role in bringing academia and industry together towards a larger goal of social good.

Vision

- ▶ To provide a focused platform and build sustained cooperation between industry and academia in the broad area of data and analytics.
- ▶ To employ mathematical, simulation, and data science tools to address problems relevant for the industry.

Mission

- ▶ The central mission of the centre is to focus on quantitative research to address problems of practical interest to the industry.
- ▶ To identify emerging trends and ideas that are of immediate practical interest.
- ▶ To maintain a sustained and active collaboration with industry for mutually beneficial outcomes.
- ▶ To plan and conduct activities that help boost research and teaching in areas of common interest – e.g., applied mathematics, data science, machine learning, high performance computing, etc.
- ▶ To promote interest and employability among students for careers in these areas.
- ▶ To foster joint activities between academia and industry.



Need for the Centre

In modern society, a significant fraction of the products and services, including business intelligence, are perfected by cutting-edge quantitative analysis. The current era, often referred to as Industry-4.0, envisages the deployment of smart and connected manufacturing and delivery systems that tightly coupled physical and digital processes. Hence, much of productivity and efficiency will result from a combination of application of mathematical, data, and AI tools.

A collaboration between IISER Pune's quantitative researchers and data-rich industries is mutually beneficial. Academics not only have the expertise to work with mathematical models and data but are constantly working with emerging ideas and trends. The industry is increasingly generating more data than ever before and seeking to benefit from it. This ranges from improved manufacturing productivity to better decision support systems. Hence, it's beneficial for academia and industry to come together to work on a range of problems around the central theme of data, analytics, and simulation.

In a short time frame of less than 20 years, IISER Pune has emerged as one of the premier institutions in India for science research. Over the years, its faculty and students have been recipients of many awards and accolades for their research output.

By launching this Centre, IISER Pune brings together its expertise in areas related, but not restricted, to applied mathematics, analytics, data sciences, computing, and simulations towards addressing industry-focused problems. This helps in forging a close collaborative work with industry to address problems that have immediate relevance in industrial settings.

The centre acts as a platform for industry - academia and industry - industry collaborations.



The activities of Centre revolve around following four pillars:

Research activities

- Industry partners can bring their research projects to the centre and seek solutions.
- Industry partners may also choose to work in a collaborative mode.
- Joint proposals in response to various national and international calls-for-proposals that appear from time to time.
- Fellowship program for postdoctoral and other researchers with relevant expertise to work on industry-focussed problems.

Visitors programme

- Hosting visiting professionals from industry for short-term engagements.
- Providing industry practitioners with in-house facilities.
- Facilitating short-term engagements for academicians in industry.

Training human resources

- The centre focuses on training the future workforce for cutting edge industry jobs. Individuals from industry and academia will benefit from the training at this centre.
- Certification courses to be launched in areas of common interest, drawing experts from IISER Pune and the industry.
- Undergraduate Research Award programme for senior undergraduate (5th year) and Masters (2nd year) students to take up internships at the centre to work on industry-focussed problems.
- The centre makes conscious efforts to encourage participation of women in scientific and industrial research.

Events and outreach

- The centre's activity includes organising industry-academia workshops, conferences and brainstorming sessions regularly.
- The centre hosts events aimed at students and also train college teachers in areas of interest of the Centre.
- Thematic Industry-academia connect events jointly with industry partners.
- Monthly seminar series by academicians and industry experts with broad national visibility.

Domain expertise

Molecular dynamics

For any industry application, simulations of complex processes are the first steps in any feasibility investigation before more expensive wet lab experiments are performed. Centre has extensive experience and expertise for carrying out large-scale molecular dynamics simulations of a variety of systems ranging from several classes of materials to biological systems. This includes simulations of proteins, DNA, protein-DNA interactions, electrolytes, polymers, etc. Even more sophisticated techniques, such as umbrella sampling, different versions of metadynamics, thermodynamic integration, etc. are carried out to obtain free energetic estimates of a process that is more accurate and match closely to experimental realisations.

Drug design

Computer-aided drug design is an integral part in the current approaches to drug design. The centre has expertise to carry out various docking studies, de novo design of drug molecules, and test them computationally using MD simulations and free energy calculations. Our groups are adept at using AI-driven tools (such as RFdiffusion, AlphaFlow, etc.) that aid in the discovery of new drugs for a particular target.

Machine learning

IISER Pune has expertise in various Machine Learning techniques. In our work, we employ deep learning, graph convolutional neural networks, LSTM, reinforcement learning, etc. We routinely develop new specialised parallel algorithms targeted towards a wide range of domains in the basic sciences as well as in applied fields. A dedicated high performance computing facility at IISER Pune caters to our infrastructural requirements.

Quantum computing

This is one of the emerging areas that promises faster and efficient solutions for certain classes of problems in a wide range of industrial settings. This could include, but not limited to, supply-chain optimisation (and also most types of optimisation) problems, privacy protection, cryptography, high-precision sensing, and communications. IISER Pune leads India's efforts in this area and has a strong faculty strength and infrastructure in nearly all these areas.



Urban data analytics

In the last one decade, many new tools and data sources such as *OpenStreetMap* have emerged that are of immense benefit in route planning and optimization, for mobile applications that require location-aware services (e.g., cab aggregators), and as a simulation tool to predict traffic and other tools of relevance in urban landscape.

Quantitative finance

Decisions related to financial transactions taken by either commoners, market participants or regulators often depend on solutions to complex mathematical and statistical problems. Those include but are not limited to fintech applications, option pricing, financial portfolio optimization, credit risk evaluation, and many others. IISER Pune has mathematical and simulation expertise and industry experience in these areas.

Weather and climate data analytics

Data analytics is an integral part of weather and climate studies. Mathematical and statistical models and machine learning approaches are used to work on problems ranging from cloud organisation, extreme heat and precipitation events and forecasting monsoon variability. Expertise in these areas will facilitate industry academia collaborations in areas such as weather forecasting, disaster risk assessment, urban heat island effects, agricultural advisory and environmental consultancy. Some of these products are useful for industries ranging from insurance to transportation.

Computational material science

Microscopic understanding of material properties is imperative for *in silico* designing of novel materials. At IISER Pune there are expertise available to carry out large-scale density functional theory (both time-dependent and time-independent) based calculations, coupled with molecular dynamics simulations of different flavours, for eg. *ab initio*, classical and quantum mechanics molecular mechanics, path integral, etc. Additionally, we have expertise in performing nudged elastic band calculations and kinetic Monte Carlo simulations. Using these tools material properties across large length scales and long time scales can be extracted for practical applications.



From data to information

In the current era of precision cosmology, international experiments are providing high quality and large volumes of data. The analysis and physical modelling of this data requires the development of computational and statistical tools at a scale that is unprecedented in order to answer fundamental questions. At IISER, we have expertise in multiple branches of this effort that can be leveraged for industry requirements: simulation techniques that employ high-performance computing through parallelisation over thousands of cores, developing novel statistical tools to extract specific patterns within the data, and applying cutting-edge machine learning techniques to optimise the extraction of useful information from the vast amounts of raw data.

Algorithms from wetware

Living systems may appear to be a soup of chemicals that interact in complex and unpredictable ways towards solving problems an animal encounters in its environment. Sub-cellular and intercellular interaction networks are wired in ways that solve many of these problems. Since these networks have evolved over billions of years, understanding how biological systems solve problems related to pattern recognition, pattern classification, navigation, memory storage and retrieval will provide insights into successful, perhaps optimal, biological algorithms to exploit complex information. We develop detailed and idealised models of neurobiological interaction networks at several scales that reveal how animals sense odours, navigate, remember, and recollect. Efforts are on to develop an electronic nose based on insect olfactory systems to detect a cocktail of volatile components in a person's breath that can be used to identify pathological states.

Quantum materials and emergent phenomena

Computational research is crucial for understanding the fundamental physics of quantum materials and designing them for applications in quantum computing, spintronics, and other advanced technologies. The IISER team specialises in advanced theoretical models and numerical simulations to obtain information about the electronic, magnetic, and topological properties of these materials. By manipulating parameters such as strain, doping, and external fields, researchers can predict material responses, guiding experimental efforts and the development of novel devices.



Associated researchers

Susmita Adhikari

Assistant Professor (Physics) | <https://rb.gy/6shsr1>

Cosmology & Astrophysics, Dark Matter Halos, Structure formation, Cosmic structure formation, Gravitational waves, Cosmic expansion and gravity, Subhalo distributions.



Amit Apte

Professor (Data Science) | <http://sites.iiserpune.ac.in/~apte>

Data assimilation problems, Hamiltonian dynamics, Dynamics of the Indian monsoon, Lagrangian data assimilation, Hamiltonian System



Collins Assisi

Assistant Professor (Biology) | <https://assisilab.github.io>

Theoretical Neuroscience, The Hippocampal formation, Olfactory system, Neuronal networks, TensorFlow, Odor mixture processing, Oscillatory synchronization, Spatiotemporal patterning, Data-driven Neuroscience



Arka Banerjee

Assistant Professor (Physics) | <https://arkabanerjee.github.io>

Computational Cosmology, Statistics and Machine Learning for Big Data in Cosmology, Physics of Dark Matter.



Apratim Chatterji

Associate Professor (Physics)
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Phase transitions and statistical physics of Soft matter systems, Soft condensed Matter, Microfluidics



Prasenjit Ghosh

Associate Professor (Physics / Chemistry - Joint)

<https://sites.google.com/view/pghosh>

Computational material science: Predictive ab initio modelling in the areas of heterogeneous catalysis, photovoltaics, thermoelectrics and hydrogen bonded molecular crystals. Development of machine learning based interatomic potentials.

Tools used: Density functional theory (DFT), Time-Dependent DFT, various flavours of Molecular dynamics, Kinetic Monte Carlo (KMC), Nudged Elastic Band (NEB).



Pranay Goel

Associate Professor (Biology) | <https://digimed.acads.iiserpune.ac.in>

Mathematical biology: physiology and type 2 diabetes, Data science and predictive modeling for healthcare and precision (personalized) medicine, Mathematical biology



Anindya Goswami

Associate Professor (Mathematics / Data Science - Joint)

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Stochastic optimal control, Portfolio optimisation, Pricing theory of derivative contracts, Machine learning model of derivative pricing, Statistical inference for asset price models, Numerical solution for PDEs.



Neena Joseph

Assistant Professor (Earth and Climate Science)

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Climate dynamics, Tropical variability, Numerical weather prediction, Predictability, Teleconnection mechanisms, Tropical intraseasonal oscillations



Mukul Kabir

Professor (Physics) | <http://sites.iiserpune.ac.in/~mukul/>

Quantum materials and emergent quantum phenomena, 2D materials and heterostructures, Magnetism and topology, Computational condensed matter and electronic structure theory



M. S. Madhusudan

Professor (Biology / Data Science - Joint)

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Bioinformatics and Structure, Modeling structures of proteins and their complexes, Structural biology, Model protein interactions, Model biological complexes



Joy Monteiro

Assistant Professor (Earth and Climate Science / Data Science - Joint)

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Climate Modelling, Physics and health impacts of extreme heat, Climate risk estimation, Extreme rainfall and its impactsClimate System, Tropical climate, Building climate model hierarchies



Arnab Mukherjee

Professor (Chemistry / Data Science - Joint)

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Theoretical and computational chemistry, Biophysics, Single water entropy, Protein DNA intercalation, Bending mechanism of organic crystals, Drug-DNA Intercalation, DNA structural change



Suhita Nadkarni

Associate Professor (Biology)

<https://sites.google.com/view/computationalneurobiologylab>

Biophysical models of synaptic plasticity in health and disease, Synaptic Morphologies, The alpha-rhythm phenomenon, Cholinergic modulation, Neurotransmission, Energy/information balance during Synaptic Transmission, Amyloid Precursor Protein (APP)



Leelavati Narlikar

Associate Professor (Data Science / Biology - Joint)

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Machine learning for healthcare, novel algorithms to learn new biology from high-throughput data



Moumanti Podder

Assistant Professor (Mathematics) | <https://rb.gy/nay6au>

Probability (including Random Graphs as models for real-life networks), Combinatorics, Stochastic Processes (including Time Series Analysis), Statistics, Statistical Mechanics, Probabilistic Cellular Automata, Probabilistic Tree Automata, Mathematical Logic on Random Graphs



M. S. Santhanam

Professor (Physics) | <http://sites.iiserpune.ac.in/~santh>

Quantum computing, Complex networks, machine learning, nonlinear and complex systems, extreme events and data-driven modelling.



Seema Sharma

Professor (Physics) | <http://sites.iiserpune.ac.in/~seema>

Experimental high energy physics, Supersymmetry, Two-Higgs-doublet models, Extended neutrino sectors, Developing algorithms for reconstruction of hadronic and electromagnetic showers, The Large Hadron Collider (LHC)



Arun Venkatnathan

Professor (Chemistry) | <http://sites.iiserpune.ac.in/~arun>

Molecular modeling, Fuel cells and computational quantum chemistry, Battery Electrolytes, Polymer Electrolyte Membrane (PEM), Carbon capture, Thermal stability, Grain Boundary formation, Effect of Polymer chain length, Charge carriers or Dopants, Lithium-ion battery electrolytes, Sodium-ion battery electrolytes



Modality of Collaboration

Individuals and Industry can become partner in this Centre through following modes:

- (a) Support through corpus creation for setting up infrastructure, research facilities and human resource required for Centre's operations. Naming opportunities available under this initiative.
- (b) Activity or project based collaborations for supporting research, consultancy, training and outreach activities through long term as well as annual grants.

Benefits for all the stakeholders :

1. Industry benefits through the expertise and facilities available at IISER Pune – faculty, post-doctoral fellows and students, research facilities, and events organised at IISER Pune.
2. Industry gets access to human resources with relevant expertise – student and postdoctoral resources – in areas of relevance to the Centre.
3. Industry can engage with academia to research and implement new ideas into their systems and processes.
4. IISER student community benefits from exposure to regular interactions with industry-based practitioners.
5. It helps IISER's research community through finding applications of their research work.

Want to interact with us ?

If you have more questions, or simply want to discuss new possibilities/ proposals or would like to initiate an activity under the aegis of Centre for Intelligent Solutions, you are most welcome to write to us at cis@iiserpune.ac.in or reach out to any of the coordinators mentioned below:

Dr. Anindya Goswami : anindya@iiserpune.ac.in

Prof. Mukul Kabir : mukul.kabir@iiserpune.ac.in

Prof. Arnab Mukherjee : arnab.mukherjee@iiserpune.ac.in

Prof. M. S. Santhanam : santh@iiserpune.ac.in

Even before taking the first step of an engagement, you may contact the coordinators for more information about its operations for instance, Non-Disclosure Agreement.







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