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The Centre for Modeling and Simulation (2003–07)

Excellence in Academics, Research, and Outreach

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We must learn to honor excellence in every socially accepted human activity, however humble the activity, and to scorn shoddiness, however exalted the activity. An excellent plumber is infinitely more admirable than an incompetent philosopher. The society which scorns excellence in plumbing because plumbing is a humble activity and tolerates shoddiness in philosophy because it is an exalted activity will have neither good plumbing nor good philosophy. Neither its pipes nor its theories will hold water.

John Gardner, Excellence, 1961

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1 Executive Summary

Purpose and Vision

- Modern Science and Technology has become increasingly interdisciplinary, and the water-tight compartmentalization of scholarship in traditional disciplines is turning out to be increasingly futile and obstructive to the growth of knowledge. A problem is a problem – it does not care about how we choose to classify it, and a solution to the problem may come from advances not necessarily any in one of the traditional domains of knowledge. Modeling of real-life situations in nature, science, technology, and industry requires certain common denominator of knowledge and training in applied mathematics, applied statistics, and computing apart from domain knowledge.
- The Centre for Modeling and Simulation is a vibrant and spirited focal point academic and research activities in this area on the University of Pune campus.
- The Centre trains students in all three aspects of modeling and simulation, and has initiated or proposed a number of innovative academic/teaching programmes, highly multidisciplinary research programmes, and outreach programmes.

Academic Programmes

- A one-year Advanced Diploma Programme in Modeling and Simulation.
- Specialized M.Sc.-level courses in computational courses.
- A proposed two-year M.Tech. Programme in Modeling and Simulation.
- A proposed two-year M.Sc. Programme in respective disciplines with specialization in Modeling and Simulation.

Research Programmes

- Computational Materials Modeling.
- Systems Biology.
- Complex Nonlinear Systems, PDEs, and Continuous Modeling.

Outreach Programmes

- Integrated Resource Centre for High-Performance Computing.
- Network Computing Services for the Campus.
- Credit Courses for Other University Departments on the Campus.
- Extramural Research Sponsored by the Centre (2003-05).
- Colloquia and Seminars for Society At Large, with a View to Promote Awareness about M&S Methodologies.

2 Vital Statistics

Faculty Strength 1 Emeritus Professor, 1 Professor, 2 Readers, 1 Lecturer, 1 Associate	6
Technical Support Staff 2 Systems, 1 Library	3
Administrative Support Staff 1 Accounts, 1 Store, 1 General	3
Research Staff (2003-07) 3 JRF, 4 SRF, 2 RA Support for Extramural Research on Campus: 2 JRFs, 3 SRFs	9
Total Number of Publications Since August 2003	25
Project Proposals (Approved/Sanctioned)	3
Project Proposals (Submitted/Pending)	3
Total Research Funding Approved + Sanctioned	Rs. 1,50,00,000
Faculty Representation in Conferences and Invited Talks	35
Academic Programmes In Operation 1, Proposed 3	4
Student-to-Research Ratio	3:1
Visiting and Guest Faculty	18
Distinguished Visitors (2003-07) International 11, National 12	23
Colloquia and Seminars Arranged (2003-07)	30

Exploration of the full range of our own potentialities is not something that we can safely leave to the chances of life. It is something to be pursued avidly to the end of our days. We should look forward to an endless and unpredictable dialogue between our own potentialities and the claims of life – not only the claims we encounter, but the claims we invent. And by potentialities I mean not just skills, but the full range of our capacities for sensing, wondering, learning, understanding, loving, and aspiring...

John Gardner, Self-Renewal, 1964

3 Introduction

3.1 Vision, Mandate, and Objectives of the Centre

The Centre for Modeling and Simulation, University of Pune, was established in August 2003 with the aid of the *University with Potential for Excellence* (UPE) funding from the University Grants Commission (UGC). Keeping up with the modern trends in academics and research worldwide, the Centre's vision and mandate is as follows:

1. To promote, support, and facilitate academic and research activities related to mathematical modeling and computational simulation and, in particular, the use of computation as the "third scientific methodology" (besides theory and experiment).
2. To aggressively promote a problem-centric outlook to real-life problems, and highly multidisciplinary approaches that transcend traditional boundaries separating individual scientific disciplines.
3. To keep up with the state-of-the-art in computing and, in particular, develop strong expertise computing technologies such as high-performance computing, grid computing, etc., and promote a culture of sophistication in computing on the University of Pune campus.
4. To establish a backbone for research and academics that cuts across disciplines, and serves as a seed for nucleation of such activities on the University of Pune campus.

Last, but not the least, is the highest and unstated mandate of all academics: to create excellent, versatile minds that are capable of learning by themselves, of thinking deeply, of questioning dogma and authority, and of seeing beyond the immediate.

3.2 What is Modeling and Simulation?

Perhaps it may not be such a bad idea to begin by elaborating on what we mean by the terms *modeling* and *simulation*.

Model, *n.* **1** a usually miniature representation of something; also : a pattern of something to be made **2** an example for imitation or emulation **3** archetype **4** a description or analogy used to help visualize something (as an atom) that cannot be directly observed **5** a system of postulates, data, and inferences presented as a mathematical description of an entity or state of affairs.

source: www.merriam-webster.com

Simulation, *n.* **1** The imitative representation of the functioning of one system or process by means of the functioning of another <a computer simulation of an industrial process> **2** Examination of a problem often not subject to direct experimentation by means of a simulating device.

source: www.merriam-webster.com

Simulation, *n.* **1** Imitation or representation, as of a potential situation or in experimental testing **2** Representation of the operation or features of one process or system through the use of another: computer simulation of an in-flight emergency **3** Attempting to predict aspects of the behaviour of some system by creating an approximate (mathematical) model of it. This can be done by physical modeling, by writing a special-purpose computer program or using a more general simulation package, probably still aimed at a particular kind of simulation (e.g., structural engineering, fluid flow). Typical examples are aircraft flight simulators or electronic circuit simulators. A great many simulation languages exist; e.g., Simula.

source: www.dictionary.com

A *model* tries to capture the essential features of a system under scrutiny. A *simulation*, on the other hand, attempts to represent a model of the system under study using some other well-understood system, the *simulation system*, wherein features of interest of the system under study are represented using properties of the simulation system. The correctness of representation of features of interest embodied by the model, and whether one system could at all be simulated by another should be the principal concerns of a "theory" of simulation. Assuming that the model did capture essential ingredients of the system being studied, and that the simulation system is capable of representing the model to sufficient accuracy, the corresponding simulation could be expected to mimic the behaviour of the underlying real-life system.

Most often, mathematics is used to model the system under study. Usually, the need to understand the system in a *quantitative* fashion and the ability to make *quantitative* predictions about the system are the key reasons for using mathematics in this fashion. From a purist point-of-view, patterns of behaviour of a system are oftentimes perceived as having some sort of inherent mathematical structure: Either deciphering that structure and expressing it in the most concise fashion, or developing a mathematical structure inspired by the observed behaviour of the system, is of great interest to some. Indeed, all scientific theories can be thought of as models representing aspects of "reality" to within their own respective domains of applicability.

Conceivably, one could attempt a naïve classification of mathematical models into two very broad classes, namely, probabilistic vs. non-probabilistic. Probabilistic (or stochastic) models, which are based on the formalism of probability theory, are perhaps the only known way to model situations where noise, randomness, complexity, uncertainty, or ignorance dominate either the behaviour of the system or the observation process. Non-probabilistic (sometimes called deterministic) models are based on the assumption of absence of these confounds.

The most challenging modeling and simulation problems arise when the system under study is neither well-understood nor, possibly, mathematized. For example, in comparison with physical systems, complex phenomena such as human social behaviour are neither as well-understood, nor are as mathematized, in microscopic detail, as physical theories. Construction of a simulation system for such phenomena may have somewhat nebulous boundaries between an art and a science. Furthermore, the bounds of validity of the mathematical model for a system have a direct influence on the reliability of the simulation system. The degree of identity (or similarity) between the behaviour of the real system and the simulated system needs to be determined so as to enable making of valid inferences based on observations of the simulated system.

A mathematical model typically extracts essential features of the system under study from the *knowledge domain*. For example, the mathematical model of air flight would have to incorporate fluid dynamical statements about the properties of air as a fluid system. A typical modern scientific team working on a challenging real-life problem consists of domain experts (e.g., experts in fluid dynamics), mathematical modeling experts, and experts from the field that is being used to construct the simulation system. In case modern digital computers are used to perform a simulation, the field of expertise for constructing a simulation system would be computer science and engineering. Other cases, for example, a full-scale flight simulation system, could involve expertise from almost every branch of engineering and robotics just to construct the simulation system.

A simulation is thus built using these three principal components; namely, (a) domain expertise, (b) mathematical modeling strategies, and (c) methodologies and technologies specific to the simulation system.

In modern times, digital computers have emerged as the preferred simulation system to perform simulations on. Usually, a mathematical model of the system under scrutiny is programmed into a computer and then run, and the behaviour of the model as observed in this simulation is used to make inferences about the real system that is being modeled and simulated. It appears that the use of computers saves costs because employing them in place of full-scale physical simulation systems reduces the engineering overheads (although the scientific principles at the base still need to be incorporated). If we choose to use a computer to perform simulations, then its behaviour and properties as a simulation system must be "well-understood": this implies that an academic programme designed around the use of computers as simulation systems of choice must have sufficient theoretical and practical content to ensure strong foundations in computation.

3.3 People at the Centre

3.3.1 Centre's Faculty Profile

Outlook on Faculty Recruitment • In the first phase of recruitment, a small but highly qualified and dedicated dedicated core faculty consisting of 2 readers and 1 lecturer (see details below) has been recruited. This core faculty was chosen with a view of building a broad-based expertise in applied mathematics, applied statistics, and computing. In the second phase of recruitment, we plan to expand the Centre's faculty strength by recruiting specialists in areas overlapping with the Centre's existing research areas (at least 3 each).

Dilip G. Kanhere • Professor of Physics, and Director, Centre for Modeling and Simulation. Ph.D. in Physics (1976, IIT Kanpur); F.A.Sc.; UGC Career Award (1981); Meghnad Saha Award for Theoretical Sciences (2005). With more than 90 publications in reputed journals to his credit, Prof. Kanhere is one of the leading computational condensed matter physicists in the Indian scientific arena. He is the mastermind who defined the vision and focus of the Centre. His current research areas include physics of materials, quantum dots, nanoparticles, and atomic clusters. He heads a dynamic research group in the Department of Physics, University of Pune, and has active collaborations with materials scientists throughout the world. Prof. Kanhere established the campus-wide network in early 1990's, and is responsible for its maintenance, up-keep, and support. Prof. Kanhere has also been instrumental in developing and establishing several large-scale and high-performance computing facilities on the University campus.

Padmakar V. Panat • Professor Emeritus, Centre for Modeling and Simulation. Ph.D. in Physics (1972, University of California at Berkeley); Prin. V. K. Joag Award for Best Teaching and Research (1996); Best teacher Award (1995, from Pune Municipal Corporation). Retired as a Professor of Physics from Department of Physics, University of Pune, Prof. Panat has joined the Centre as a Professor Emeritus. Highly respected as a teacher of physics and mathematics, Prof. Panat has much to offer to his students; notably, a wide perspective on physics, mathematics, and natural sciences in general, a strong social outlook, and a high-degree of infectious enthusiasm. Prof. Panat is the author or co-author of several textbooks; namely, a book on Electrodynamics, a 2-volume book on applied science for engineering students, and a book on classical mechanics. He has more than 50 research publications to his credit.

Prashant M. Gade • Reader, Centre for Modeling and Simulation. Ph.D. in Physics (Nonlinear Dynamics and Complex Systems; 1993, University of Pune). Dr. Gade's research interests include Chaotic and complex systems, and computational biology. He has 22 research publications with a collective citation number of around 200. Prior to joining the Centre as faculty, Dr. Gade travelled widely across the world and held various research and faculty positions at institutes such as ICTP (Italy), JNC (Bangalore), HKBU (Hong Kong), Academia Sinica (Taipei, Taiwan), Ohio University (Athens, USA), and BITS (Pilani). He is a regular referee for the journals IJCNN, Chaos, Physica A, Physica D, Physical Review E, Pramana and Physical Review Letters. He has been an invited speaker in national and international conferences.

Sukratu Barve • Lecturer, Centre for Modeling and Simulation. M.Tech. in Materials Science (1995, IIT Mumbai), Ph.D. in Physics (General-Relativistic Quantum Field Theory; 2002, TIFR, Mumbai). Prior to joining the Centre as a faculty in 2006, Dr. Barve worked as a faculty at the Birla Institute of Technology and Science (Goa Campus), as a visiting scientist at the Albert Einstein Institüt Max Plank Institüt für Gravitationsphysik, Golm, Germany, and as a postdoctoral researcher at the Institute of Mathematical Sciences, Chennai, and the Physical Research Laboratory, Ahmedabad. Highly valued at the Centre for his analytical and mathematical skills and his passion for teaching, he is the only oddball at the Centre who has resisted, so far, the urge to resort to computation using computers. Dr. Barve's native research interests include general theory of relativity and quantum field theory on curved spacetime (areas in which he has 8 research publications in prestigious journals) and nonequilibrium statistical physics. His BITS experience has widened the scope of his research to include industrial and real-life problems in areas such as diffusion in zeolites, granulation processes, and applications of computational fluid dynamics (CFD). As a personal quest, Dr. Barve has an enormous interest in history (especially that of the city of Pune) and human geography, where he intends to apply his considerable analytical skills, mathematical expertise, and the M&S approach.

Mihir Arjunwadar • Reader, Centre for Modeling and Simulation. Ph.D. in Physics (Computational Condensed Matter; 1996, University of Pune). After a brief postdoctoral stint at the University of Pune, Dr. Arjunwadkar held a research computing position for several years at the Statistics Department, Carnegie Mellon University, an experience that opened up his mind to the fascinating world of signal plus noise. He has 14 research publications to his credit, one of which (in collaboration with Christopher R. Genovese, Christopher J. Miller, Robert C. Nichol, and Larry Wasserman of Carnegie Mellon University) has received the American Statistical Association's Outstanding Application Award for 2005. His current research interests include development of computational methodologies for challenging problems, statistical data modeling and analysis, computational condensed matter and statistical physics, complex systems, and computational/systems biology. Specifically, he has an on-going collaboration with Dr. Sanjeev Galande, National Centre for Cell Science (NCCS), Pune, in the area of systems biology and bioinformatics.

3.3.2 Visiting and Guest Faculty

Outlook on Visiting Faculty • The Centre actively welcomes experts from academics, research, and industry as visiting and guest faculty so as to maximize the exposure of our students to a wider world. The Centre also provides active logistic support for international visitors who would like to visit the Centre for time periods from a few days upto a year. In 2006, the Centre invited Dr. William B. Sawyer (see details below) for a 4-month visit. Close interaction with Dr. Sawyer was an enriching experience for our students. It has also opened possibilities of international collaborations for the faculty, and of an international project for students.

William B. Sawyer • Chakraborty Software GmBH, Zürich, Switzerland. Visiting Scientist (August–December 2006), Centre for Modeling and Simulation. Dipl. Inf. Ing. in Computer Science Engineering (1987, ETH Zürich); M.S. in Scientific Computing/Computational Mathematics (1993, Stanford University); Doctor of Sciences in Mathematics (2006, ETH

Zürich). After his M.S. degree, Dr. Sawyer worked in the field of algorithm development for high-performance computers at the Swiss Center for Scientific Computing (CSCS, Manno, Switzerland) and at NASA Goddard Space Flight Center (Greenbelt, MD, USA). He returned part time to the ETH Zürich for doctoral studies in 2001, and completed his thesis "Efficient Numerical Methods for the Shallow Water Equations on the Sphere" in 2006. His main research interests are in modeling global atmospheric dynamics on supercomputers, and software frameworks for Earth Science applications. He has 11 peer-reviewed publications in journals such as Numerische Mathematik and International Journal for High Performance Computer Applications.

Abhijat Vichare • Researcher at CFDVS, IIT Powai. Guest faculty (2005-06), Centre for Modeling and Simulation. Ph.D. in Physics (Computational Condensed Matter; 1997, University of Pune). Dr. Vichare's research interests include theory of computation, formal verification, compiler construction, and functional programming.

V. Sundararajan • Group leader, Scientific and Engineering Applications Group, C-DAC. Guest faculty (2005-07), Centre for Modeling and Simulation. Ph.D. in Physics (Computational Condensed Matter; 1994, University of Pune). Dr. Sundararajan now heads a large group within C-DAC. His research interests include materials modeling, genetic other evolutionary algorithms, traffic modeling, and machine learning.

K. C. Sharma • Professor Emeritus, School of Space and Atmospheric Sciences, University of Pune. Guest faculty (2005-07), Centre for Modeling and Simulation. Formerly a faculty at the Defence Institute of Advanced Technology (DIAT), Prof. Sharma is an applied mathematician with extensive experience in partial differential equations, computational fluid dynamics, and their real-life applications.

U. V. Naik-Nimbalkar • Professor of Statistics, University of Pune. Guest faculty (2005-07), Centre for Modeling and Simulation. Prof. Naik-Nimbalkar's research work is focussed on inferences in stochastic process, survival analysis, and reliability.

S. G. Kunte • Retired Professor of Statistics, University of Pune. Guest faculty (2005-07), Centre for Modeling and Simulation. Prof. Kunte, a pedagogue par excellence, specializes in Bayesian inference.

V. K. Jayaraman • Scientist F, Chemical Engineering Division, NCL. Guest faculty (2006-07), Centre for Modeling and Simulation. Prof. Jayaraman's research focusses on applications of machine learning methods to chemical engineering problems.

A. P. Gore • Professor of Statistics, University of Pune. Guest faculty (2005-06), Centre for Modeling and Simulation. Prof. Gore is a highly respected name in the field of biostatistics, known for his originality, authenticity, and a strong social dimension to his research work.

S. B. Gokhale • Professor of English, University of Pune. Guest faculty (2006-07), Centre for Modeling and Simulation.

Niraj Dudani • Researcher, National Centre for Biological Sciences, Bangalore. Guest faculty (2006-07), Centre for Modeling and Simulation.

Ashutosh • Persistent Systems Pvt. Ltd. Guest faculty (2005-07), Centre for Modeling and Simulation. Ph.D. in Physics (Fluid Dynamics; 1997, University of Pune). Dr. Ashutosh has extensive experience in scientific software development in the corporate world. His research interests include turbulence, complex systems, bioinformatics, and machine learning.

A complete list of our guest and visiting faculty can be found on the Centre's website at `http://cms.unipune.ernet.in/people/guest/`.

3.3.3 Centre's Staff Profile

Abhay Parvate • Programme Coordinator, Centre for Modeling and Simulation. M.Sc. in Physics (1997, University of Pune). Mr. Parvate is a mathematical physicist and a graduate student at the Department of Physics, University of Pune, working on his Ph.D. thesis in the area of calculus on fractals. Mr. Parvate is the strong backbone that keeps the everyday operations related to the Centre's *Advanced Diploma Programme in Modeling and Simulation* on the track, in addition to which, he is also responsible for teaching computing-related courses. A first-class programmer by passion, Mr. Parvate's other passions include system administration, software engineering, organization of anything and everything that he happens to run into (people, disc and office space, computing resources, and knowledge), and singing in his office.

Neeta Kshemkalyani • System Administrator, Centre for Modeling and Simulation. M.Sc. in Computer Science (Scientific Computing; 1999, University of Pune). Ms. Kshemkalyani has a long experience in managing all aspects—technical, human and administrative—of the University-wide network consisting of about five thousand machines organized into many sub-networks, in building Beowulf computing clusters, and in keeping various high-performance platforms such as the SGI Altix 3700 owned and managed by the Centre up and running.

Administrative and Other Staff • The strong backbone of the Centre's daily and mundane operations is the Centre's efficient and able administrative and library staff, namely, **Alka Chaudhari** (library), **Mrunalini Dharmadhikari** (office), **Ashok Nikale** (store), and **Neelima Khilare** (accounts). Our cleaning lady, **Kalabai Mundinkeri**, has a silent yet significant presence all through the Centre's premises.

A former staff who left the Centre very recently, **Rajendra Sasane**, *needs a special mention here: for the first two years of Centre's existence, Mr. Sasane, with his qualification of only a higher-secondary certification examination, took care of all administration – from small errands to elaborate accounts operations – in a single-handled, seamless, and efficient manner. This example not only illustrates what an excellent mind capable of learning could achieve in a short span of time, it also shows how excellence in administration could be realized in a non-hierarchical organizational setup and a serious yet flexible work culture.*

3.3.4 Centre's Student Profile

Abhijeet Sonawane • M.Sc. in Physics (2005, University of Pune). Mr. Sonawane works with Dr. Gade as his Ph.D. advisor and Dr. Goswami (BARC) as his experimental collaborator in the area of nonlinear dynamics of coupled laser arrays.

M. Ali Saif • M.Sc. in Physics (2005, University of Pune). Mr. Saif works with Dr. Gade as his Ph.D. advisor in the area of complex systems and econophysics.

Sameet Mehta • M.Sc. in Zoology (2001, University of Pune). Mr. Mehta, formally registered as a graduate student at the National Centre for Cell Science (NCCS), works in collaboration with Dr. Arjunwadkar. His Ph.D. research in systems biology and bioinformatics has the unique feature that it attempts to combine wet-lab biology with computational modeling.

Students in the Advanced Diploma Programme • Although too numerous to be listed here, our students in the *Advanced Diploma Programme in Modeling and Simulation* are the vibrant life force at the heart of the Centre. Their native backgrounds range from M.Sc. (mathematics, statistics, physics, etc.) to B.E. (chemical, computer, biotechnology, etc.).

3.4 Infrastructure at the Centre

3.4.1 Computing Facilities

High-Performance Computing Facilities for the Campus Community • The Centre manages and maintains high-performance computating resources for the entire campus community. These facilities include:

- A SGI Altix 3700, a 16-processor (Intel Itanium) SMP platform with 32GB of single-image RAM, and over a TB of disc space.
- A Bull machine, another 16-processor (Intel Itanium) SMP platform with 32GB of single-image RAM.
- A large linux cluster consisting of 16 node, 32 processors, and 64 cores (Intel Xeon Woodcrest) with infiniband interconnects. This will become operational by mid-May 2007.

In-House Computer Network • The Centre has an in-house fully-networked computational laboratory for its students, currently consisting of 20 desktops plus supporting equipment such as a 20KVA UPS, two large split AC units, a printer, etc. The Centre's computer network is primarily `linux`-based, and boasts of a large scientific software base. Every member of the Centre, including students, staff, and faculty, has been provided with an individual desktop for productivity[1].

3.4.2 Library

The Centre has an in-house library that boasts of a hand-picked collection of about 1000 books. In addition, the Centre's library has subscriptions to newspapers and magazines of general interest in addition to technical periodicals.

3.4.3 Web Presence

The Centre's simple yet elegant and functional website came into existence in early 2004. Unlike many fancy websites that remain in their initial state almost forever, the Centre's website is a constantly growing website with new material added regularly and frequently. It is no wonder that the Centre's website is one of the most frequently visited websites on the University of Pune campus network. All members of the Centre, including students and staff, get their own personal web space in the Centre's webpage hierarchy, an encouragement to express themselves through this medium, and sufficient initial technical know-how for a first step.

The Centre is perhaps a pioneer (on the University of Pune campus) in the methodical use of its website for pedagogic purposes. Although the Centre is yet to deploy a sophisticated course management system such as `DotLRN`, it has experimented extensively with the use of webpages as an instructional aid and as a yet another medium for communication between students and instructors. For instance, a completely anonymous and unmoderated online course feedback mechanism for students was deployed right at the inception of the *Advanced Diploma Programme in Modeling and Simulation.*

On a technical note, unlike many websites on the University of Pune network, the Centre's website boasts of technically clean and valid `html` sources.

[1]The only known exception to this rule is our cleaning lady.

3.4.4 Building

Although plans for the Centre's very own building were ready as early as in 2004, the actual construction work is likely to commence only in mid-2007 for reasons entirely unknown to, and beyond the control of, the Centre. During 2003-04, the Centre was physically located in the Department of Physics, University of Pune. The Centre moved to its current location on the top floor of the Computer Science Department, University of Pune during 2005-06 at the commencement of the first batch of the *Advanced Diploma Programme in Modeling and Simulation*.

3.5 Organizational Structure, Work Culture, Ethos

The Centre has an almost non-hierarchical organizational structure. Artificial divisions or labels such as students, staff, faculty are entirely functional in nature and devoid of any value judgment or vanity associated with them. The Centre harbours and protects a completely informal and flexible, yet serious, work culture. Disagreements are not discouraged, and regimentation is not encouraged. Independent, original thought, authenticity, creativity, initiative, and entrepreneurship are highly encouraged in all aspects of the Centre's functioning, and in all members of the Centre. Individuality of others is not only respected, it is fiercely protected. The willingness to explore uncharted territories and untrodden paths is, again, highly encouraged. Such a work culture and environment that is devoid of stress, frustration, and resentment is believed to bring out the best in any individual member of an organization, and thereby lead to excellence at individual and collective levels.

All logistic support for maximizing productivity is provided. Such support includes, e.g., flexible work hours, and a 24-hour access (for members of the Centre) to the Centre's premises, offices, and facilities. The decision-making process at the Centre is democratic and collective (over appropriate subsets of the Centre's members). Non-critical decisions are often made in an off-line fashion, i.e., over email[2].

[2] The Physics Department is a pioneer within the University in this respect, to the best of our knowledge.

We don't even know what skills may be needed in the years ahead. That is why we must train our young people in the fundamental fields of knowledge, and equip them to understand and cope with change. That is why we must give them the critical qualities of mind and durable qualities of character that will serve them in circumstances we cannot now even predict.

John Gardner, Excellence, 1961

4 Academics at the Centre

4.1 Ground Realities of Indian Undergraduate Education

In our collective experience of past two decades or so as teachers, we observe that the great Indian undergraduate education system, on the average, serves to effectively curb independent thinking, self-study skills, resourcefulness, intellectual maturity, academic confidence, and the very motivation to learn with excellence. Academic excellence is often identified, wrongly, with performance in examinations that tend to assess mostly memorization skills of a student, and the true measures of academic excellence such as depth of understanding, originality, authenticity, creativity, and perseverance are systematically discouraged.

While the reasons for this deplorable situation could be traced all the way back to Indian primary education, it is generally agreed that the immediate cause for the situate is the disproportionate importance that end-semester or end-year examinations have come to attain, starting right from the secondary and higher secondary school certificate examinations. This is seen to encourage, on the average, unhealthy learning styles on part of the students. For example, mindless memorization instead of an understanding of the underlying principles of a topic is usually perceived by students as the most successful strategy for "getting through" an examination. To make the situation worse, students coming typically from rural areas unnecessarily feel hampered by their self-perceived lack of proficiency in English.

As a thin silver lining to this dark cloud, a small respectable minority of students somehow survives through the damages inflicted by the great Indian undergraduate education system. The reasons for this are not entirely clear to us, but very likely they are related to strong family values or a local culture/environment that encourage excellence, and perhaps because of excellent, dedicated teachers at various levels who took their job seriously.

By the time a student enters a post-graduate programme in a University, he or she is usually under the additional pressure of finding either a career or an assured well-paying job (the latter expectation is further inflated in times of economic boom such as the present one). To make things worse, it turns out that many students have never been exposed to the notions of excellence, authenticity, and commitment to quality, and are generally confused about their goals.

The purpose of a University is "to give the society what it *needs*, and not what it *wants*"[3]. While it could be argued that the effort to institute remedial measures for this social malady should ideally exist in the very structure and ethos of a University, we believe that, in its absence, independent effort at all levels should be encouraged.

On a completely different note, we have witnessed a considerable rise over the past decade in the proportion of students with stringent family commitments–children, in particular. This is clearly a reflection of the transitions in the urban social structure in the modern times. A common characteristic of such students is their strong motivation to learn and improve their qualification while trying to balance their personal lives, without much support from their extended families or the society at large. A University should ideally provide a positive support and moral reinforcement to such students. This will very likely require fundamental reforms in the very structure, ethos, and outlook of an average or typical Indian University.

The academic programmes designed by the Centre are vigorous and demanding programmes if implemented in their true spirit. We see these realities as the greatest confound in the effective deployment of any serious academic programme. Indeed, some of the experiments and remedial measures initiated by the Centre have been discussed in Sec. 4.4.

[3]Edsgar W. Dijkstra, *The Strengths of the Academic Enterprise*, 1994. Emphasis ours.

4.2 The Centre's Outlook on Higher Education

The Centre's outlook on higher education[4] could not have been better-expressed than what John Gardner wrote in his seminal 1961 book *Excellence: Can We Be Equal and Excellent Too?*:

We don't even know what skills may be needed in the years ahead. That is why we must train our young people in the fundamental fields of knowledge, and equip them to understand and cope with change. That is why we must give them the critical qualities of mind and durable qualities of character that will serve them in circumstances we cannot now even predict.

This insight is perhaps even more pertinent now than back in 1961, considering the accelerated rate of change of technology that has resulted into overall faster timescales of change in the social, economic, scientific, and technological domains. It could be reasonably argued that such "durable qualities of character" should include versatility, resourcefulness, and the very ability to learn, to improve oneself, and to keep up with the changing world in a continuous manner.

As a general rule, the Centre attempts to strongly encourage excellence in all aspects of its operation, and attempts to inculcate in its students qualities that the Indian undergraduate education effectively manages to destroy. In particular, the Centre strives to promote and sustain the true qualities of academic excellence, namely, originality, resourcefulness, independent thought, depth of understanding, authenticity, creativity, perseverance, and tenacity.

4.3 Curriculum Design and Development Initiatives

Over the past four years, the Centre has come up with innovative curriculum designs for four novel programmes; this section outlines these curriculum design initiatives. Detailed programme documents for the first two programmes below are publically available on the Centre's website `cms.unipune.ernet.in`. Highlights of our curriculum designs, our outlook on pedagogy, and operational aspects are as follows:

- Highly modular structure conducive to resource-sharing across departments.
- A student-to-teacher ratio of about 3:1, and readily accessible faculty. This makes possible to monitor student progress closely, and to do mentoring and counselling on a regular basis.
- Effective, optimal combination of time-tested classroom teaching, student-teacher interaction, modern educational technologies for off-line learning, and hands-on work.
- Full access to the Centre's premises and facilities.
- Continuous assessment of students.
- Student intake from diverse backgrounds, from mathematics and science, to engineering[5].
- Placement support for projects and jobs. Currently established notable contacts in this area include ETH, Zürich, Switzerland (via Chakraborty Software, Zürich, Switzerland), Tech Mahindra, and Motorola Labs India.
- Specialized courses run in collaboration with campus departments and industry.

[4] Actually, this applies equally to education at all levels.

[5] In principle, even arts, commerce, or management backgrounds are acceptable provided a certain minimal mathematics background can be guaranteed.

4.3.1 Advanced Diploma Programme in Modeling and Simulation

The *Advanced Diploma Programme in Modeling and Simulation*, which was designed during 2004, became operational in AY 2005-06. This is a highly-interdisciplinary one-year post-graduate full-time diploma programme that attempts to impart a systematic and thorough training in all three foundations of mathematical modeling and computational simulation, namely, applied mathematics, applied statistics, and computing. The programme year is broken up into three trimesters. The first two trimesters are devoted to coursework consisting of core courses and an elective. The third trimester is devoted entirely to project work. The programme curriculum is supplemented by colloquia and seminars aimed at generating a perspective on modeling and simulation in general, and domain-specific problems, applications, methodologies.

Detailed description of this programme can be found on the Centre's website at
`http://cms.unipune.ernet.in/programmes/2005-06/sam.pdf`,
`http://cms.unipune.ernet.in/programmes/2006-07/curriculum/`
and
`http://cms.unipune.ernet.in/programmes/2006-07/syllabus.pdf`.

Similarly, a list of colloquia and seminars arranged by the Centre can be found at
`http://cms.unipune.ernet.in/announcements/archive.shtml`.

4.3.2 Master of Technology (M.Tech.) Programme in Modeling and Simulation

Our *Master of Technology (M.Tech.) Programme in Modeling and Simulation* is currently awaiting approval from the University of Pune. It will become operational after the Centre moves to its own building and premises, possibly during AY 2008-09, and after acquiring additional faculty strength and resources.

Aims and Objectives. This programme is a unique, fast-paced, and vigorous academic training programme that aims at creating a breed of problem-solvers

- who have a breadth and perspective on mathematical modeling, a solid training in simulation methods, impeccable computational skills, and the ability to generate reasonable solutions, algorithmic or otherwise, for problems not necessarily encountered earlier;
- who are familiar with the current state of relevant technologies, and from familiar to skilled in a variety of relevant software tools and methodologies; and
- who, outside of their native knowledge domain, have sufficiently broad background and skills to interface between domain experts and coders in a multidisciplinary team.

Academic Structure. This is a highly interdisciplinary programme that focuses on mathematical modeling formalisms and simulation methodologies by integrating applied mathematics, statistics, and computing in a coherent package. This is *not* a programme in the traditional domain of computer science. This programme may, however, be thought of as a *computational science* programme.

This programme consists of core and elective courses, and a project. In the full-time mode, the duration of the programme is 2 years (4 semesters). Each semester is broken up into 18 weeks of instruction, 1 week for preparation, and 1 week for actual end-semester examinations. The first year is devoted to coursework consisting of core and elective courses. Evaluation is based on (a) continuous assessment throughout a semester, and (b) an end-semester examination. The second year is devoted to a one-year full-time project. Evaluation of the project is based on continuous assessment, a project report, and a presentation cum open defence.

Part-Time and Distance-Learning Modes. The academic structure of the programme is flexible enough so that it could in principle be run in full-time, part-time, and distance-learning modes. With additional faculty, manpower, and resources, it may be possible to run the programme in a part-time or distance-learning mode. The part-time and distance-learning modes will make the programme most attractive to working individuals in the industrial and corporate sector, and R&D organizations.

4.3.3 Proposed Master of Science (M.Sc.) Programme in Computational Finance

This is an innovative cross-disciplinary programme, currently in its design and development phase. This programme is expected to cater to a sparsely populated, high-demand niche in the financial world; namely, financial analysts who are well-versed in modeling and simulation methodologies in addition to the fundamentals of economics and finance. Indeed, although the Centre does not have any in-house expertise in the areas of economics and finance, the motivation for this programme came from our contacts with companies and individuals in the financial and corporate world. This programme thus attempts to combine the considerable computational and M&S expertise available at the Centre with domain expertise in the area of finance and economics. Evidently, this programme can be deployed only with the help of institutes and organizations in the region who have expertise in economics, finance, insurance, etc. Apart from University of Pune Departments such as Economics and Statistics, such organizations in and around Pune include the National Insurance Academy, and companies such as Capital Metrics and Risk Solutions (`http://www.capmetrics.com/`).

The programme is envisioned to produce graduates with rigorous foundation in mathematical modeling and economics of financial markets combined with a detailed knowledge of business practices and behavioural aspects. The programme is designed to offer a quantitative and specialized training in finance that is technically much more advanced than what is typically offered in an MBA programme, but without the considerable research component of a Ph.D. Students will be learning basic portfolio theory, asset and option pricing, corporate finance, and international financial management. However, an important component of the programme is an introduction to econometric methods and data analysis.

To gain a proper understanding of modern analytical and quantitative techniques, students will be given rigorous training in areas of applied mathematics such as linear algebra, multi-variable calculus, optimization theory, probability theory, and stochastic processes. Modeling, analysis, and decision-making in economic and financial systems involves well-established analytical procedures which have opened the avenue for employing computational tools. More recently, powerful computational tools have provided the ability to proceed in novel directions. New computational developments in stochastic methods, genetic algorithms, neural networks for the modeling and control of dynamical systems have enhanced our understanding of complex models of economic behaviour such as learning and equilibria. We seek to prepare the student to acquire these skills as well. On a pedagogic note, although the topics above could also be taught in a rigorous way suited for a mathematics course, the corresponding courses are expected to begin with examples and financial models familiar to the students and abstract therefrom.

4.3.4 A Novel Cross-Disciplinary Master of Science (M.Sc.) Programme (Proposed)

We are also working on a novel cross-disciplinary multi-department collaborative Master of Science (M.Sc.) Programme. The current conception of this programme is that a student, after gaining advanced one-year training in a specialized domain area where quantitative reasoning is potentially useful or plays a significant role (such as physics, statistics, mathematics, economics, sociology, linguistics, etc.), gets trained at the Centre for one year in modeling and simulation methodologies, computing technologies, and advanced domain-specific computational methods. The Masters degree awarded to a student at the successful completion of this programme will be appropriated titled as, e.g., "M.Sc. in Sociology with Specialization in Modeling and Simulation". This programme is inspired by the proliferation, due to availability of inexpensive computing technologies, of quantitative reasoning and computational methodologies in all domains of academics and research, and of knowledge, scholarship, science, and technology.

A multi-department academic programme such as this evidently needs close collaboration and cooperation between multiple departments. After completing a thorough ground-work, the Centre plans to approach various departments on the University of Pune campus to assess their interest in this programme.

4.4 Student Support

4.4.1 Continuous Monitoring, Mentoring, and Counselling

The Centre has a faculty-to-student ratio of about 1:3. The Centre's faculty is highly accessible to the students. A student's progress is monitored on a continuous basis. All faculty engages in student counselling very regularly, which makes it possible to identify issues at an early stage and to take proactive measures before a problem blows up out of proportion.

An Anonymous Feedback Mechanism • Specifically, a completely anonymous web-based mechanism for feedback on a course or an instructor has been deployed at the very inception of the *Advanced Diploma Programme in Modeling and Simulation* in AY 2005-06.

Orientation Sessions • The Centre has also initiated the practice of arranging orientation sessions for newly admitted students at the beginning of every academic year. This way, they get a clear picture of what to expect during their tenure at the Centre, and are mentally better-prepared for the it.

Planning Ahead • The Centre's core team religiously attempts to plan an academic year well ahead of time in as detailed manner as possible, and to take proactive measures for foreseeable eventualities as best as possible. This makes it possible for everybody at the Centre to have a clear idea of the academic year ahead, and to plan their own activities in a better fashion.

4.4.2 Value Addition and Soft Skills

Creative Thinking • Motivated by the issues highlighted in Sec. 4.1, the Centre has experimented with the unconventional and innovative approach. As a proof-of-concept experiment, the Centre organized a Workshop on Creative Thinking primarily for its students, but generally for all interested staff and faculty. This 3-day workshop was conducted in December 2006 by Mr. Sharad Sunkar, an expert in the field who has been conducting such workshops in the corporate world for last 20 years or so. We believe that this experiment has been quite successful; we have witnessed a general boost in the resourcefulness and productivity of our students, and they are better able to cope up with the pace of the *Advanced Diploma Programme in Modeling and Simulation*. We also believe that given the availability of a qualified psychologist with effective communication and personal skills and a speciality in creativity training, such results should be reproducible with a large probability across batches of students.

Time Management • As yet another experiment in a similar vein, the Centre organized for the students informal sessions on effective time management by people who are masters of that art. Two most prominent speakers for these sessions were Dr. William B. Sawyer, who visited the Centre during August–December 2006, and Dr. Sanjeev Galande, National Centre for Cell Science (NCCS).

4.4.3 Keeping Up the Morale of Socially Challenged Students

The Centre's faculty and staff are exceptionally sensitive to, and supportive of, highly motivated students who wish to strike the difficult balance between personal lives and responsibilities on one hand, and their academic or career aspirations on the other. This is in response to a family support system of olden times that is failing with the fast-changing nature of an urban socioeconomic system, and the extraordinary drudgery of everyday life in an infrastructurally challenged urban setting of an average Indian city like Pune.

4.4.4 Placement Support

One of the most frequent queries from potential candidates in our *Advanced Diploma Programme in Modeling and Simulation* has been the placement record of the Centre's students. To this end, the Centre has initiated placement activates for our students[6]. Specifically, the following measures have been initiated by the Centre so far:

- Organization of presentations and counselling sessions conducted by experts on opportunities and career possibilities in relevant domains.
- Industry contact initiatives for project placements, with the eventual goal or hope of being absorbed in relevant organizations, companies, etc. Such formal or informal contacts have been established with a number of companies or organizations; here is an indicative sample in alphabetical order:

Capital Metrics & Risk Solutions	`www.capmetrics.com`
C-DAC	`www.cdac.in`
Chakraborty Software (Zürich, Switzerland)	`www.chakraborty.com`
Golden Embryo Technologies	`www.goldenembryo.com`
In Silico Consulting	`www.insilico-consulting.com`
MSC Software	`www.mscsoftware.com`
Motorola Labs India	`www.motorola.com/in`
Persistent Systems	`www.persistent.co.in`
SAS India	`www.sas.com`
Tech Mahindra	`www.techmahindra.com`
Tata Research Development and Design Centre	`www.tcs-trddc.com`

Activities that are under consideration for implementation include:

[6] Indeed, our students have benefitted greatly from the extensive expertise generously shared by our neighbours, the placement cell of the Computer Science Department, University of Pune.

- Arranging showcase events and campus interviews with initiative generated from the students' side.
- Formation of a formal placement cell at the Centre, to be operated entirely by the students to coordinate all placement-related activities[7]. All required logistics support could be provided by the Centre. The Centre's placement cell could operate, to a mutual benefit, in collaboration with two existing initiatives with a long history at two other departments, namely, the Computer Science Department, and the Interdisciplinary School of Scientific Computing.
- Arranging pertinent activities such as workshops on designing a resumé, writing cover letters, appearing for interviews, etc., via the placement cell.

4.5 M&S Colloquia

The curricula (Sec. 4.3) in modeling and simulation developed by the Centre's academic team, by design, focus almost exclusively on methodological aspects of modeling and simulation. It is highly essential to impart to the students a perspective on modeling and simulation that will bring together this diverse set of concepts into a unified view, both from conceptual and practical points of view. Domain knowledge at some level is assumed on part of the student and, depending on the elective, may be enhanced to some extent in the course of these programmes. What is missed upon in these curricula is a perspective on modeling and simulation field as a whole (and, specifically, the "art" aspects of modeling and simulation) that will bring together the diverse set of concepts, methodological or otherwise, into a unified view, both from conceptual and practical points of view.

To remedy this situation, the Centre has resorted to arranging colloquia, seminars, and case-study sessions by experts from industrial or academic research domains, with the intention of generating a perspective on current real-life applications of modeling and simulation as a methodology. By a *seminar*, we mean a specialized and focussed presentation on a research topic. A *colloquium* is a relatively extended presentation that is aimed at a lay, non-expert, or mixed audience, is usually biased towards the pedagogic end (as opposed to the "research" end) of the spectrum, and does not assume–generally–any domain-specific expertise on part of the audience. A *case-study* is a focussed and somewhat longer (3-6 hours) session with a strong hands-on component, presented and coordinated by an expert. The purpose of the M&S colloquia, seminars, and case-study sessions is twofold:

1. To illustrate the art of (mathematical) modeling in practice.
2. To generate a perspective on, and increase awareness about, modeling and simulation as a methodology.

In our experience, such a perspective could be generated in two distinct ways:

1. By exposing the audience to a variety of applications and examples from diverse areas of science and technology that employ modeling and simulation as a methodology, and by imparting a clear understanding, at an appropriate level of detail or description, of
    - the underlying scientific or technological system or problem, and the complexities in it;
    - the modeling decisions that went into building an appropriate mathematical model for this system or problem;

[7]Ideally, the University of Pune needs a well-organized Career Resource Centre with a humane face that is readily accessible to the entire campus community.

- the (mathematical) complexity of this model, and possible ways of extracting useful information from the model;
- the need to resort to computation and simulation, and the complexities involved therein;
- what is learnt about the system or problem through modeling and simulation, and how well does the model corroborate with real life.

2. By presenting an overview, at an appropriate level of detail or description that depends on the audience, of one or more *open* problems in a field where modeling and simulation methodologies are likely to help.

In addition, a focussed tutorial on a specific computational tool or environment (e.g., the `ns-2` network simulator, the `phoenix` software for computational fluid dynamics, etc.) could also serve as a case-study session.

A society whose maturing consists simply of acquiring more firmly established ways of doing things is headed for the graveyard – even if it learns to do these things with greater and greater skill. In the ever-renewing society what matures is a system or framework within which continuous innovation, renewal and rebirth can occur.

John Gardner, Self-Renewal, 1964

5 Research at the Centre

5.1 Computational Materials Modeling

The present focus of research of the computational materials modeling group headed by Prof. Dilip Kanhere is on the physics of subnano systems. This group uses atomistic modeling using *ab initio* density functional methods. Typical properties investigated include:

1. Finite-temperature properties of clusters like Gallium and Tin. Al, Na, Au cages and impurity systems like Ti in Si_{16} cages. These studies are motivated by recent observations of unusually extreme size-sensitivity and higher-than-bulk melting points.
2. Magnetic properties of clusters of Mn and MnAs.
3. Interaction of gold clusters with acetone.
4. Physics of confined electron systems; e.g., quantum dots.

This research group needs and uses the high-performance computing facilities of the Centre extensively.

5.2 Systems Biology

Systems Biology, a 21st century integrative approach to biology, seeks to understand[8]

the workings of biological systems as a whole, placing a greater emphasis on the interactions between components, and the consequences of such interactions, than on the components themselves (which, in a post-genomic era, are largely known)... Systems Biology can be summarised as the science of analysing and modelling genetic, macromolecular and metabolic networks in order to explain the higher order behaviour and function of complex systems. The hallmarks of systems biology are that it seeks to be quantitative, integrative, and synthetic – approaches that complement the more qualitative analytical strategies of pre-genomic biology.

Modelling and simulation form an integral part of the predictive and explanatory approach to systems biology. Such models can be used to produce in silico behaviours that can be repeatedly compared with those observed through experimental validation. By these means, it should be possible to form a quantitative understanding of the interactions between elements of the system (and their relative importance), to predict which experimental manipulations might prove most rewarding and, ultimately, to discover the true organisation and in-vivo behaviour of the system of interest.

The systems and computational biology research activity at the Centre was initiated through a research collaboration between Dr. Sanjeev Galande, National Centre for Cell Science (NCCS), Pune, and Dr. Mihir Arjunwadkar at the Centre. The general research focus of Dr. Galande's group at NCCS is chromatin structure and regulation of gene expression. Dr. Mihir Arjunwadkar's speciality relevant to this research focus includes large-scale numerical and scientific computing, and statistical data modeling and analysis. The most attractive feature of this collaboration is that it attempts to integrate computational modeling with wet-lab biology with a focus on solving real-life problems in the biological domain.

A research proposal titled *Systems Biology of Global Regulatory Networks: Unravelling Sequence Features in Promoters that Dictate Tissue-Specificity of Gene Expression* has been submitted to the Department of Biotechnology, Government of India, awaiting final approval for a total funding of Rs. 1,50,00,000 to be shared between NCCS and the Centre.

Activities of this research group will be expanded in the future in a variety of ways. For example, we would like to start a computational and systems biology discussion forum

[8] `http://www.bbsrc.ac.uk/science/areas/ebs/themes/main_sysbio.html`

to provide a first-rate but accelerated education in biology to people from quantitative disciplines such as statistics, mathematics, and physics, and entice them to take up problems of relevance to real biology. We would also like to expand our group by involving statisticians on the University campus who have expertise in microarray data analysis.

5.3 Complex Nonlinear Systems, PDEs, and Continuous Modeling

In last decade, physicists and applied mathematicians have been involved in analysis of 'Complex Systems'. Several natural, artificial and abstract objects and networks have been studied in this regard. These include human economies, nervous systems, power grid, food webs, organization of firms and so on. These systems are complex in several ways. Their models, however simple, can seldom be treated analytically and we have to resort to computational study. Memory, feedback loops and complex connectivity need to be embedded even in the simplest of the models. Often, tools from nonlinear dynamics and statistical physics are useful in analysing these systems.

Complex systems have involved tools like coupled map lattices which can be viewed as partly discretized partial differential equations. Tools from continuous models like PDEs have been useful in other areas related to engineering, finance and basic sciences. A few partial differential equations (PDE) are known to have wide applicability; examples are the Navier-Stokes equation, Black-Scholes equation, diffusion and population balance equations. Such equations indicate mechanisms of natural processes and are of a few types. They being applicable in a variety of ranges and contexts, offer predictive power which is precise enough for many diverse applications.

This research group consists of two faculty at the Centre, namely, Dr. Sukratu Barve, and Dr. Prashant Gade. It has submitted 10 research papers in this area in last 4 years, of which 6 have been published and 4 are undergoing a review.

Dr. Gade has ongoing active collaborations with Dr. Limaye's group in Department of Physics, Prof. Sudeshna Sinha in Inst. of Math. Sci. in Chennai, Prof. Somadatta Sinha in Centre for Cell and Molecular Biology and Prof. B. K. Goswami from BARC in Mumbai. There are two Ph.D. students working in this group. Dr. Gade has given lectures in NIAS (Bangalore), TIFR (Bombay), Dept. of Phys. (Pune) and an invited lecture in conference SMPRI in Bangalore on these works.

Similarly, Dr. Barve has ongoing active collaborations with Dr. S. Jhingan, Centre for Theoretical Physics, Jamia Millia Islamia University, New Delhi, and Dr. S. Krishnaswamy, Department of Chemical Engineering, BITS-Goa, Zuarinagar, Goa.

Some of the specific focus areas of this group are described below:

1. Wealth Distribution in Human Economies. The fat tail in wealth distribution in Human economies has been a puzzle for long. In a couple of works, we have shown that it could be explained using simple agent based asset exchange models.

2. Coupled Neuronal Systems. The coherent and synchronous activities in neuronal systems are linked to unhealthy situations like epilepsy and Parkinson's disease. Using simple models of neurons, we have published a work which attempts to understand the origin of coherent dynamics in coupled neuronal system.

3. Coupled Maps on Networks. Several of the features of coupled oscillator models could be reproduced in coupled maps. We are continuing a program on exploring dynamics of such systems on variety of networks, coupling schemes and presence of feedback. Cellular automata and combinatorial methods have been employed in some of the examples above.

4. Partial Differential Equations and Non-Analytic Behaviour. We are exploring the behaviour of nonlinear PDEs in situations wherein non- analytic behaviour of the dependent variable is seen. In particular, this is known to occur in a general relativistic context near curvature singularities. We have explored a particular example which involves rotation in the background manifold (spacetime). Certain methods for handling the non-analyticity had to be adapted for this model. This led to results which could be interpreted in the domain of general relativity as regards initial data and evolution. We are seeking to apply similar techniques to situations of dynamical phase transitions and other nonequilibrium phenomena.
5. Pattern Formation. Pattern formation is another area where PDES have been useful especially in the discretized form as coupled map lattices and cellular automata. Discrete agents interacting with each other and a background resource could be viewed from this angle, and one can study the resulting patterns. There are two particular phenomena which are being considered, viz segregation and extinction. We are proposing a generalized principle of competitive exclusion which basically says that the patterns which compete for the same resource remain segregated when the resource is small. We are proposing a dynamical model of extinction on lines of Bak-Sneppen model.
6. Partial Differential Equations in Engineering. We are addressing various applications of continuum mechanics in diverse engineering contexts ranging from diffusion in zeolites to granulation in chemical engineering. Tools for computational fluid dynamics and computational structural engineering are being set-up for this purpose. We have planned to validate simple models with existing data from industry.

If the man in the street says, "Those fellows at the top have to be good, but I'm just a slob and can act like one" – then our days of greatness are behind us. We must foster a conception of excellence that may be applied to every degree of ability and to every socially acceptable activity. A missile may blow up on its launching pad because the designer was incompetent or because the mechanic who adjusted the last valve was incompetent. The same is true of everything else in our society. We need excellent physicists and excellent mechanics, excellent cabinet members and excellent first-grade teachers. The tone of our society depends upon a pervasive and almost universal striving for good performance.

And we are not going to get that kind of striving, that kind of alert and proud attention to performance, unless we can instruct the whole society in a conception of excellence that leaves room for everybody who is willing to strive – a conception of excellence which means that whoever I am or whatever I am doing, provided that I am engaged in socially acceptable activity, some kind of excellence is in my reach.

John Gardner, Excellence, 1961

6 Centre's Outreach Programme

6.1 Credit Courses for Other University Departments

All Centre's academic programmes have a highly modular structure, a *module* being the smallest logical unit of instruction. This makes it possible to offer individual modules to interested students of other departments on the campus, provided class schedule at the other department is not in conflict with at the Centre, and provided the student's background satisfies any prerequisites for such a course/module offered by the Centre. Centre's courses and modules are advertised on the Centre's website well ahead of time. Since the commencement of our *Advanced Diploma Programme in Modeling and Simulation*, our courses and modules have been taken by students at the following departments on the campus:

- Department of Physics,
- Department of Environmental Sciences, and
- Institute of Bioinformatics and Biotechnology (IBB).

The Centre has also organized joint courses in specialized topics of common interest (such as machine learning and high-performance computing) in collaboration with the following departments on the campus:

- Department of Computer Science, and
- Interdisciplinary School of Scientific Computing.

6.2 Services for the Campus Community

The Centre manages and maintains a SGI Altix 3700 as a high-performance computational resource for the entire campus community that is available upon request. This machine is a 16-processor (Intel Itanium) SMP platform with 32GB of single-image RAM, and over a TB of disc space. Another computing platform with a similar configuration, a Bull machine, is also managed by the Centre. A large beowulf cluster consisting of 16 Dell nodes (dual core dual xeons–total of 64 cores, infiniband interconnects, etc.) has recently been purchased by the Centre. Once operational, this cluster will also be available as a shared resource to the campus computational research community.

6.3 Extramural Research Sponsored by the Centre

Following the mandate of promoting interdisciplinary research involving modeling and simulation, the Centre invited research proposals from University of Pune faculty in AY 2004-05. The support provided by the Centre was five JRF fellows for a period of one year and computer time on computing facilities managed by the Centre. Six research proposals were received from physicists, statisticians, and a psychologist of the campus. After conducting interviews of about 20 candidates, 4 were selected to work on four of these projects, and 2 actually joined their positions. This included the research in psychology. Additionally, the Centre has supported 3 SRFs in the Department of Physics for a period of 6 months during AY 2003-04, and 2 RA positions for 3 years. Currently, the Centre supports 1 SRF and 1 JRF to work with Centre's faculty.

Complete details of the AY 2004-05 project proposals can be found on the Centre's website at `http://cms.unipune.ernet.in/announcements/2004-08-16-2359/`

6.4 Society At Large

The M&S Colloquia (see Sec. 4.5) and seminars organized by the Centre are an open event for interested public at large, with a view of generating awareness on modeling, simulation, and computation as the "third scientific methodology" besides theory and experiment. These events are methodically advertised across the University campus, at relevant institutes, organizations, and industry in the region, and over a large and growing voluntary electronic circulation list maintained by the Centre. The M&S colloquia have especially been well-received by lay audience. Our selection of speakers includes highly accomplished and internationally acclaimed experts in diverse fields.

Complete details of colloquia and seminars organized by the Centre can be found on the Centre's website at `http://cms.unipune.ernet.in/announcements/`

When organizations feel they need an infusion of new talent, they look to their recruitment process. But the largest untapped reservoir of talent is in people already recruited but thereafter neglected.

The quickest road to renewal is the mining of that untapped resource. Among other things it would solve the problem of maintaining an organization that is responsive to both leaders and the people it serves. Vital people, using their gifts to the full, are naturally responsive. People who have stopped growing, who no longer have confidence in the use of their own powers, build bastions of procedure.

John Gardner, US Civil Service Commission Anniversary Speech, 1996

7 The Future of the Centre

7.1 Sustained Excellence Needs Sustained Stability: Continued UGC Support is Crucial

The current UPE support for the Centre will formally come to an end on March 31, 2007 (March 31, 2008, in case the UGC grants a 1-year extension sought by the University). We appreciate this support that gave us an opportunity to experiment with many innovative ideas, design novel academic programmes, and tread on new walks of research. We would, however, point to the issue of long-term stability of the Centre and similar other institutes and centres established in an *ad hoc* fashion.

With the exception of the Director of the Centre (who is a professor of physics formally affiliated to the Department of Physics, University of Pune), all the current faculty at the Centre have been hired on a 5-year contract basis. In our judgement, there is no possibility that the state government will ever take over the Centre as a granted department.

The uncertainty surrounding the future of the Centre is quite demoralizing to all members of the Centre. This is especially true for the contract faculty (even though their contracts are to expire in about two years time, in or around year 2009). Indeed, it should be noted that the current faculty joined the Centre because of the lure of an enticing concept and a promise of innovation on which the Centre is founded, and not because they could not have secured positions elsewhere.

This is not a healthy situation, despite the fact that the current faculty is highly motivated and dedicated to research and academics. It is not very clear to us whether the question of long-term future of such *ad hoc* centres and departments was considered *prior* to establishing them. Nevertheless, if the Centre is to be firmly established as a centre of excellence and is to continue to flourish, then the University and the UGC need to be serious about this situation. A humane resolution of the situation in reasonable time is perhaps the only direction to take.

In the rest of this section, We first present, in Sec. 7.2, a vision for the Centre's future; namely, an outline of how the Centre would like to expand its activities in the near future. This vision is based on the key assumption that the Centre continues to survive beyond the current deadline of the UPE funding. Finally, we present a general discussion, in Sec. 7.3, on issues in promoting and sustaining excellence in a University.

7.2 A Roadmap for the Centre's Future

7.2.1 Critical Faculty Strength

Any focussed research or academic setup of the modern kind usually needs a certain critical faculty strength to develop a vigorous and dynamic intellectual ambience and sustained overall productivity. It should not be too hard to realize that although the Centre's current faculty is highly motivated, qualified, and dedicated, the overall faculty strength at the Centre is too low. Many of the activities proposed in this section could not be initiated so far partly because of lack of adequate faculty strength.

In the first phase of recruitment, a small but highly qualified and dedicated dedicated core faculty consisting of 2 readers and 1 lecturer was recruited. This core faculty, whom we refer to as *generalists*, was chosen with the vision of building a broad-based expertise in applied mathematics, applied statistics, and computing.

In the second phase of recruitment, we plan to expand the Centre's faculty strength by recruiting specialists in areas overlapping with the Centre's existing research areas (at least 3 in each). We expect that the total faculty strength at the Centre to reach about 12-15.

7.2.2 Building

Although plans for the Centre's very own building were ready as early as in 2004, the actual construction work has not commenced yet, for reasons entirely unknown to, and beyond the control of, the Centre. During 2003-04, the Centre was physically located in the Department of Physics, University of Pune. The Centre moved to its current location on the top floor of the Computer Science Department, University of Pune during 2005-06 at the commencement of the first batch of the *Advanced Diploma Programme in Modeling and Simulation*.

The scope of the Centre's activities will expand considerably once it is relocated to this new building[9]. In particular, the Centre will then be in a position to start the *Master of Technology (M.Tech.) Programme in Modeling and Simulation* outlined in Sec. 4.3.2.

7.2.3 A Shared Computer Laboratory for the Campus Community

The proposed building plan has a novel feature, namely, a computer laboratory big enough to harbour about 100 desktops. The vision for this laboratory is that, once fully set, it will be available to campus departments by prior booking for running their own computational courses. The logistic burden of managing and maintaining the infrastructure and computational setup of this laboratory will be borne by the Centre.

7.2.4 High-Performance Computing Infrastructure

The Centre plans to expand the existing high-performance computing infrastructure considerably over the next five years. Indeed, much of the current computing facilities are expected to be outdated over the next five years given the rapid pace of technology.

7.2.5 Enhancements to the Centre's Website

In the near, foreseeable future, the Centre's library catalogue will go online via our website.

While Indians are known to be avid users of open-source software, India's contribution to the open-source movement remains a contentious issue. Although the Centre is not in a position to contribute to the open-source movement at the moment, we plan to support it by setting up mirrors for a variety of open-source, public-domain software including, but not limited to `CRAN`, `CTAN`, and a range of linux distributions.

Finally, the Centre plans to deploy a sophisticated course management systems (such as `DotLRN`) that will enable instructors to deploy offline learning mechanisms in an effective manner without the aid or interference of system administrators, and a much greater overall level of automation of course management logistics.

7.2.6 Academics

With the completion of the Centre's own building, the Centre plans to start the proposed *Master of Technology (M.Tech.) Programme in Modeling and Simulation*. With an expansion of the Centre's faculty resources, other academic programmes outlined in Sec. 4.3 can be initiated as well.

7.2.7 Research

Over last four years, research at the Centre's has evolved from a loose collection of individual research problems to a consolidation into focussed research areas. The Centre plans to

[9] We have been told that the building may be ready by end of 2008.

expand its research activities by adding specialized faculty in these core research areas outlined in Sec. 5. The Centre will also consider expanding in additional research areas with a promise, such as computational finance, computational fluid dynamics, etc.

7.2.8 The Virtual M&S Journal

We plan to start a virtual internet-based research journal dedicated to modeing and simulation. Keeping in line with the Centre's vision, we envisage this journal to promote and advocate a multidisciplinary, problem-centric approach. This will be a peer-reviewed journal. At present, we are in the brainstorming stage for this project.

7.2.9 Outreach

The Centre would like to see its outreach programme strengthened and expanded to include a greater handshake with the industry, summer internship programme, programmes for undergraduates and school children to expose them to modeling and simulation ideas, etc. We have also been considering the possibility of designing domain-specific computational courses (e.g., multi-scale materials modeling) in collaboration with engineering institutes to promote a multidisciplinary approach to problem-solving.

For the campus community, the Centre plans to offer specially designed computational courses for disciplines that are traditionally considered to be on the qualitative side, such as biology, sociology, etc. The Centre also looks forward to a greater collaboration with similar-minded campus organizations, departments, and centres.

7.3 Promoting and Sustaining Excellence in the University

7.3.1 Sustained Excellence Needs Excellent Support Structures

What does it take to be a good administrator?
A, a good heart, and
B, the ability to tell if the other person is trying to take advantage of you.

J. Robert Dorfman[10]*, Personal Communication, 2003*

Collective excellence in academics needs support structures that put academics at a University before everything else, and recognize that academics is, in fact, the precondition for their very existence. In particular, the administration of this University needs massive organizational reforms to make it more responsive to the needs of academics, and to give it a human and humane face at all levels.

As the flip side of the same coin, people that constitute such support structures need to be excellent and reasonably happy in their own line of work. Bringing a human face to the support structures implies, e.g., the following:

- The human dignity of people that constitute such support structures at all levels, from those at the top to sweepers, peons, students, and faculty, is respected and protected.

  Specifically, self-sustaining measures, at personal and organizational levels, for weeding out sources of frustration need to be deployed. At the personal level, such measures originate spontaneously if people are sensitive, sensible, responsive, and devoid of vested interests.

[10] J. Robert Dorfman is a physicist at the University of Maryland renowned for his work on the foundations of statistical physics. He was an administrator for over a decade.

- Personal initiative, entrepreneurship, and effort towards making the support structure better should be positively reinforced. Such initiatives could be in the areas of, e.g., enhancing administrative efficiency, simplification, building greater responsiveness towards “customers”.

  This implies that all structures that encourage regimentation need to be reformed in a fundamental fashion.

- The University as a whole should be perceived by its members as a *beneficial* organization that allows and encourages them *to grow*, in every conceivable sense of the word. Measures to make it so could include, e.g., proactive measures to support members in the fast-changing, infrastructurally challenged socioeconomic setup of modern urban Pune.

  This also includes a better support for students, such as counselling, hostels (modeled after, say, the IITs or the IISc), excellent academic resources including a library that welcomes them.

7.3.2 Bringing Excellent Minds to the University

Collective excellence requires excellent minds at all levels in the collective. The problem of faculty attrition in academics has taken on new dimensions with the current rapid rate of expansion of the Indian economy, and the highly incommensurate pay structure across sectors (industry vs. academics, private vs. public, etc.). Many disciplines that never encountered this problem before are facing it now on a routine basis.

To make the problem worse, it appears that a major proportion of a whole generation of academic people that contributed to the growth of the University over last three decades is about to retire over next five years or so.

This situation is perhaps unique in the history of this University, and points to the need for creative solutions and innovative ways of enticing fresh talent to academics and research and for retaining them in the University system.

7.3.3 Fundamental Issues Need Fundamental Resolutions

The observations in the previous sections point to some of the most fundamental issues in the very structure and functioning of the University. The roots of these issues could be traced all the way back the Maharashtra Universities Act that established this University in the first place, and to the controlling interests of politicians in the state. It is imperative that if this University is to flourish *with excellence*, it needs much greater autonomy and a freedom from political interference to be able initiate new fundamental measures and creative practices to cope up with the fast-changing nature of the modern era.

Continued support given by the UGC under the UPE programme has gone a long in addressing some of the issues mentioned here, and is crucial for sustaining quality academics in the University of Pune.