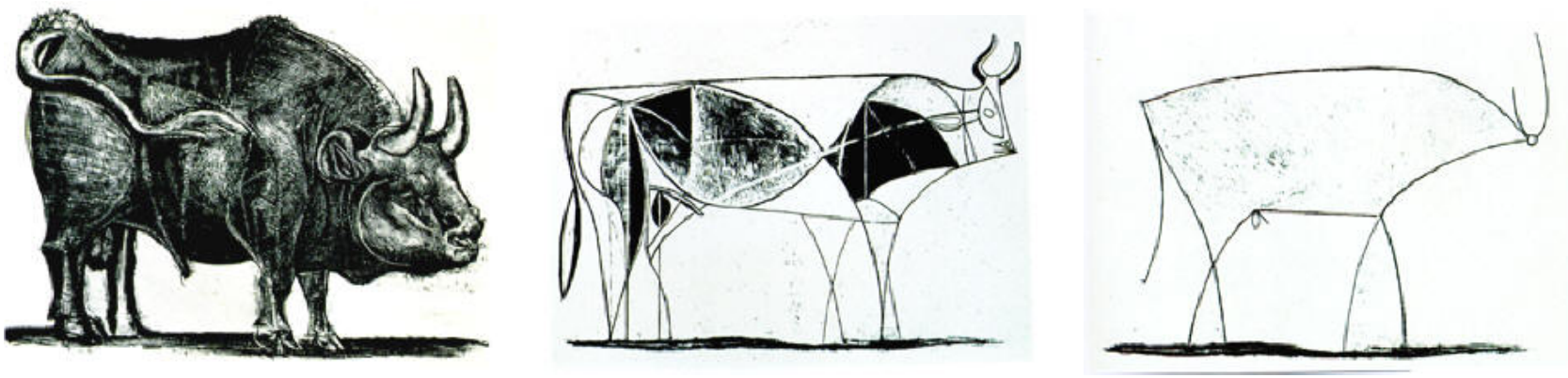
The Centre for Modeling and Simulation (2003-07)

Excellence in Academics, Research, and Outreach

Dilip G. Kanhere
Centre for Modeling and Simulation
University of Pune

March 16, 2007



The Essence of Scientific Modeling According to Picasso

Introduction

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

Vision, Mandate, Objectives

- Promote, support, and facilitate academics and research related to mathematical modeling and computational simulation.
- Promote use of computation as the "third scientific methodology".
- Promote a problem-centric outlook to real-life scientific and technological problems.
- Promote highly multidisciplinary approaches that transcend traditional boundaries separating individual knowledge domains.
- Develop strong expertise in state-of-the-art computing technologies (high-performance computing, grid computing, etc.).
- Promote a culture of sophistication in computing on the University of Pune campus.

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Academic Staff

Dilip G. Kanhere
Professor and Director

Padmakar V. Panat
Professor Emeritus

Sukratu Barve
Lecturer

Abhay Parvate
Programme Coordinator

Prashant Gade
Reader

Mihir Arjunwadkar
Reader

Sailaja Krishnamurty
Postdoctoral Research Associate

Support Staff

Neeta Kshemkalyani
Computing

Alka Chaudhari
Library

Ashok Nikale
Store

Mangesh Patil
Computing

Mrunalini Dharmadhikari
Administration

Neelima Khilare
Accounts

Visiting and Guest Faculty

William B. Sawyer
ETH, Zürich

Anil P. Gore
Statistics, UoP

S. G. Kunte
Statistics, UoP

T. V. Ramanathan
Statistics, UoP

S. B. Gokhale
English, UoP

K. C. Sharma
Space and Atmospherics, UoP

Ashutosh
Persistent Systems

R. N. Pralhad
Defence Institute of Advanced Technology

V. Sundararajan
C-DAC

V. K. Jayaraman
National Chemical Laboratory

- **Many More, + A Number of Distinguished Visitors.**

Infrastructure at the Centre

- **In-House Computing Facilities.**

  20-PC linux-networked lab for students, large scientific software base, individual PCs for all staff, full internet access for all, web space for all.

- **In-House Library.**

  A hand-picked, growing collection of $\sim$ 1000 books. Subscriptions to newspapers and magazines of general interest, plus technical periodicals.

- **Substantial Web Presence** (`cms.unipune.ernet.in`).

  Simple yet elegant, fully functional, well-maintained, and growing website. One of the most frequently watched website on the campus.

- **Building.**

  Plans approved as early as in 2004. Expected Completion: 2008.

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University-Wide Resources Managed by the Centre

High-Performance Computing Facilities for Campus Community

- **A SGI Altix 3700.**

  16-processor (Intel Itanium) SMP platform, 32 GB single-image RAM, disc space $>$ 1 TB.

- **A Bull Machine.**

  Another 16-processor (Intel Itanium) SMP platform, 32 GB single-image RAM.

- **A Large Linux Cluster.**

  16 nodes, 32 processors, and 64 cores (Intel Xeon Woodcrest), 4–8 GB RAM per node, infiniband interconnects. To be operational by mid-May 2007.

- **Campus Network Services.**

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Organizational Structure, Work Culture, Ethos

- **Almost Non-Hierarchical Organizational Structure.**
- **What is Encouraged?**

  Openness, independence, original thought, authenticity, creativity, initiative, entrepreneurship. The willingness to explore uncharted territories and untrodden paths.
- **What is Discouraged?**

  Shoddiness and regimentation.
- **Decision Making.**

  Collective and Democratic.
- **Strong Moral+Logistic Support for the Socially Challenged.**

Academics and Outreach

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

Teaching Programmes

- **Advanced Diploma Programme in Modeling and Simulation**

  More about this in the next slide.

- **M.Tech. Programme in Modeling and Simulation**

  Proposed and submitted to the University.
  Expected start date: AY 2008-09.
  Pre-requisite: Centre's own building.

- **M.Sc. Programme in Computational Finance**

  Under review by experts.

- **A Novel M.Sc. Programme with Specialization in M&S**

  1 year in a domain department + 1 year with us.
  Curriculum design project in the brainstorming stage.

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Advanced Diploma Programme in Modeling and Simulation

- **The Programme**

  A fast-paced, rigorous, one-year, post-B.E. or post-M.Sc. interdisciplinary programme. Operational since AY 2005-06.

  Student-to-Teacher Ratio: $\sim 3:1$

- **Core Courses**

  Applied mathematics, applied statistics, computing.

- **Electives**

  Domain- or methodology-oriented; e.g., computational fluid dynamics, machine learning, computational materials modeling, ...

- **Project/Industrial Training**

  Minimum 4-months. Highly encouraging response from industry.

- **100% Placement Record**

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Value Addition, Soft Skills, Student Support

- **Workshop on Creative Thinking**
  A 3-day proof-of-concept workshop conducted in December 2006 by Mr. Sharad Sunkar, an expert in the field who has been conducting such workshops in the corporate world for over 20 years.
- **Technical Communication and Presentation**
  Inclusion of a regular course in the curriculum, realizing the importance of this soft skill.
- **Time Management**
  Informal lectures by people with an in-depth perspective on time management.
- **Placement Support**
  Lectures by experts on opportunities in a variety of fields. Active formal contact with industry and other organizations.
- **Other Student Support**
  Anonymous web-based feedback mechanism. Continuous monitoring, mentoring, and counselling. Orientation sessions for the newly admitted students. Keeping up the morale of socially challenged students.

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M&S Colloquia and Seminars

Date	Speaker	Title
2007-03-14	Susana Gomez	Designing an Evolutionary Optimization Algorithm to Characterize Naturally Fractured Oil Reservoirs
2007-03-12	Arto Teras	Grids – Computing and Collaboration
2007-03-08	Susana Gomez	Global Optimization to Predict the Production of Water and Oil Reservoirs
2007-02-12	O. K. Anderson	Why Electronic Structure Calculations?
2007-02-03	Vinand Arabale	Finite Element Analysis
2007-01-08	Ranjan Mehta	Modeling Combustion Using CFD
2006-12-11	Julius Jellinek	Some Conceptual Aspects of Thermodynamics and Dynamics of Finite Systems
2006-11-25	Sanjeev Galande	Time Management: Perspectives and Strategies
2006-03-13	B. D. Kulkarni	Asymptotic Methods in Modeling and Simulation
2006-03-01	Kamlesh Pande	CFD & Modeling: Industrial Applications
2006-02-01	Pradip	Colloidal Processing of Alumina-Zirconia Composites: ...
2006-01-25	Milind G. Watve	Cooperating with Cheaters Around: New Insights into an Old Problem
2006-01-18	Vivek Ranade	Reactor, Process and Product Engineering via Flow Modeling
2005-12-22	Tanusri Saha Dasgupta	First-Principles Study of Phase Stability in Alloys
2005-12-12	Arjan K. Shahani	Mathematical Modelling for Health Care and Health Services
2005-10-26	V. Sundararajan	Modeling and Simulation of Proteins
2005-10-19	Somdatta Sinha	Modeling Biochemical Pathways
2005-02-04	Mahendra Khandkar	Orientational Ordering of Hard Rods in 2-D
2005-01-06	Ruth Lynden-Bell	Room Temperature Ionic Liquids: Simulation, Solvation and Surfaces

M&S Colloquia and Seminars

Date	Speaker	Title
2004-11-19	Prashant Gade	Dynamics on Networks
2004-10-08	Uttara Naik-Nimbalkar	Stochastic Models in Finance
2004-06-18	Sagar A. Pandit	Atomistic Simulations of "Raft" like Nano-Domains in Lipid Bilayers
2004-03-31	Julius Jellinek	Electronic, Structural and Thermal Properties of Clusters
2004-03-19	Vaishali Shah	Computational Studies of Nickel Corrosion
2004-03-05	Ankita Saxena and Ashutosh	Immunology for Dummies
2004-03-01	Uma Ramakrishnan	Understanding the Past and Predicting the Future: Insights from Population Genetic Models
2004-02-20	Dilip G. Kanhere	Thermodynamics of Finite-Size Systems
2004-01-30	Ashutosh	Making Spider Silk Protein Sequences

Strengthening Academics on the University Campus

- **Our Courses are Open to the Campus Community**
  - Our courses and modules are open to students of other campus departments (subject to constraints of prerequisites and logistics).
  - Taken by students from Department of Physics, Department of Environmental Sciences, and Institute of Bioinformatics and Biotechnology.
- **Collaborative Courses and Other Academic Activities**
  - Department of Computer Science, Interdisciplinary School of Scientific Computing, C-DAC.

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Research

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

Collective Expertise and Outlook

Collective Expertise

- High-performance computing and large-scale numerics.
- Statistical data modeling and analysis.
- Nonlinear and complex systems.
- Computational materials modeling.
- Mathematical physics and general relativity.

The Centre Strongly Encourages

- Basic and applied research for real-life problems.
- The problem-centric approach to research.
- Cross-disciplinary research that cuts across traditional boundaries.
- Collaborations with industry and specialized academic institutes.

Focus Group: Computational Materials Modeling

- **Research Focus and Outlook**

  Physics of sub-nano systems, atomistic modeling using *ab initio* density functional methods. Extensive use of high-performance computing facilities at the Centre.

- **Specific Problem Areas**

  Finite-temperature properties of clusters like Gallium and Tin. Al, Na, Au cages and impurity systems like Ti in Si_{16} cages. Magnetic properties of clusters of Mn and MnAs. Interaction of gold clusters with acetone. Physics of confined electron systems; e.g., quantum dots.

- **People**
  - Dilip G. Kanhere and his group,
  - Sailaja Krishnamurty, Postdoctoral Researcher at the Centre.

- **Collaborators**
  - Steve Blundel, France, and
  - Julius Jellinek, Argonne National Laboratory, US.

Focus Group: Computational and Systems Biology

Systems Biology, a 21st century integrative approach to biology, seeks to understand the workings of biological systems as a whole. A hallmark of systems biology is its extensive use of M&S methodologies.

- **Research Focus and Outlook**

  Application of M&S to chromatin structure and related problems in a biologically useful manner. Close handshake between computational and wet-lab approaches.

- **Specific Problem Areas**

  Unravelling sequence features in promoters that dictate tissue-specificity of gene expression. Innovative adaptation of methodologies from other domains, e.g., statistical mechanics, complex systems theory, statistical genomics.

- **People**
  - Mihir Arjunwadkar, the Centre, and
  - Sameet Mehta, a graduate student at the Centre.

- **Collaborators**
  - Sanjeev Galande, National Centre for Cell Science, Pune.

A shared research funding of 1.25 Crores is awaiting final approval from DBT.

Focus Group: Complex and Nonlinear Systems

- **Research Focus and Outlook**

  Theory of complex and nonlinear systems, and its applications to real-life problems.

- **Specific Problem Areas**

  Wealth distribution in human economies. Coupled neuronal systems. Pattern formation. PDEs in engineering and non-analytic behaviour. CFD.

- **People**
  - Sukratu Barve and Prashant Gade, the Centre, and
  - Abhijeet Sonawane and M. Ali Saif, graduate students at the Centre.

- **Collaborators**
  - Abhay Limaye, Department of Physics,
  - Sudeshna Sinha in MatScience, Chennai,
  - Somadatta Sinha, CCMB, Hyderabad,
  - B. K. Goswami, BARC, Mumbai,
  - S. Jhingan, Jamia Millia Islamia, New Delhi, and
  - S. Krishnaswamy, BITS-Goa, Goa.

A Roadmap for the Future

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. ...

John Gardner, Self-Renewal, 1964

Critical Faculty Strength

- **Current Faculty Strength**
  - 2 Readers, 1 Lecturer *(apart from 1 Professor and 1 Emeritus)*
  - Highly motivated and dedicated *generalists* recruited with the vision of building a broad-based expertise in applied mathematics, applied statistics, and computing.
- **Vision for Recruitment Phase II**
  - Focussed research/academic setup needs a certain critical faculty strength to develop a vigorous and dynamic intellectual ambience and sustained overall productivity.
  - Recruit ~ 3 *specialists* each in the three research focus areas.
  - Expected total faculty strength at the Centre: 10–15.

Academics

- **M.Tech. Programme in M&S**
  - Programme awaiting approval by the University.
  - Prerequisites: Enhanced faculty strength, Centre's own building.
- **Collaborative Academic Programmes with Other Campus Departments**
  - For example, "M.Sc. in Physics with Specialization in M&S".

Research

- **Strengthening of Existing Research Groups**
  - Add $\sim$ 3 specialized faculty in each area.
- **Expansion in Related Research Areas**
  - At a brainstorming stage.
  - Possibilities: computational finance, computational fluid dynamics.
- **The Virtual M&S Journal**
  - A peer-reviewed, internet-based journal dedicated to computational science, modeling and simulation.
  - To promote and advocate a multidisciplinary, problem-centric approach. This will be a peer-reviewed journal.
  - This project is in the brainstorming stage at present.

Outreach

- **A Shared Computer Laboratory for the Campus Community.**
  • Capacity $\sim$ 50-100 desktops, available to campus departments by prior booking for running their own computational courses.
  • Logistics, management, and maintenance: by the Centre.
  • Prerequisite: Centre's own building.
- **Computational Courses for Specialized Audiences.**
  • For disciplines traditionally considered *qualitative*.
  • In collaboration with engineering institutes to promote a multidisciplinary approach to problem-solving.
- **Programmes for Undergraduates and School Kids.**
  • Summer internships, etc.
- **Greater Handshake with Similar-Minded Organizations and Industry.**

The Centre's Whereabouts

Web **http://cms.unipune.ernet.in/**

Phone +91.(20).2569.0842
+91.(20).2569.1140
+91.(20).2560.1401

Fax +91.(20).2569.1684

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