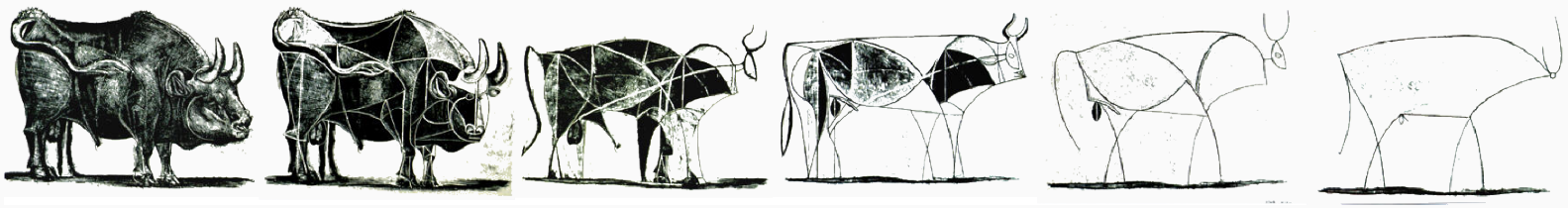
Centre for Modeling and Simulation

. . . because all models are false and some are useful . . .

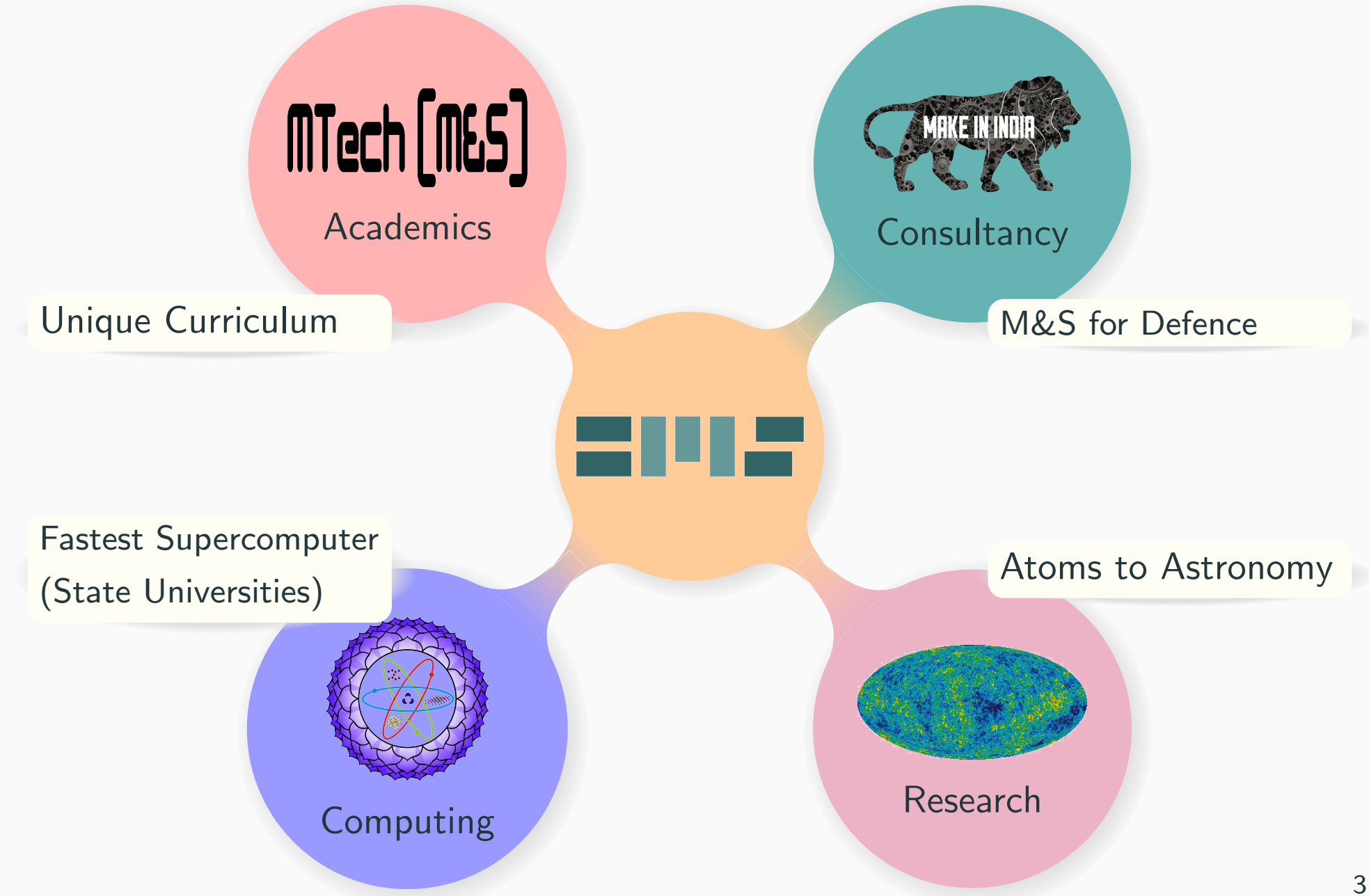
January 21, 2017



. . . I was impressed to hear that this Centre was started in the early 2000s, when such places were still rare even in the U.S., and to see the multi-disciplinary projects that take place there. I hope that this Centre continues to thrive . . .

– Dr. Rebecca McNamee (GIAN Faculty) to Hon'ble Vice Chancellor, 2016

CMS in a Nutshell



Vision

Established in 2003 through UPE seed funding from UGC, to

promote modeling and simulation methodologies

encourage and support truly multi-disciplinary, problem-centric approaches to basic and applied research

transcend traditional boundaries separating knowledge disciplines

Details (p.29) | A Cartoon Guide to M&S (p.51)

Faculty and Staff

- Director (Additional Charge)
- Associate Professor: 1 (Contract)
- Assistant Professors: 3 (1 UGC FRP, 2 Contract)
- Postdoctoral Fellows: 4 (2 DS Kothari, 2 DST NanoMission)
- Academic/Placement Coordinator: 1
- Administrative & Technical: 5

Details (p.31) | Awards & Recognitions (p.32) | Visiting Faculty (p.33)

Infrastructure

Highlight: High-Performance Computing

- **Sahasrar**: 1000+ Intel cores, 50 nodes

(Possibly) fastest+largest amongst state universities

- **Ashtanga**: ∼100 Intel cores, 8 nodes
- Other smaller-scale computing clusters

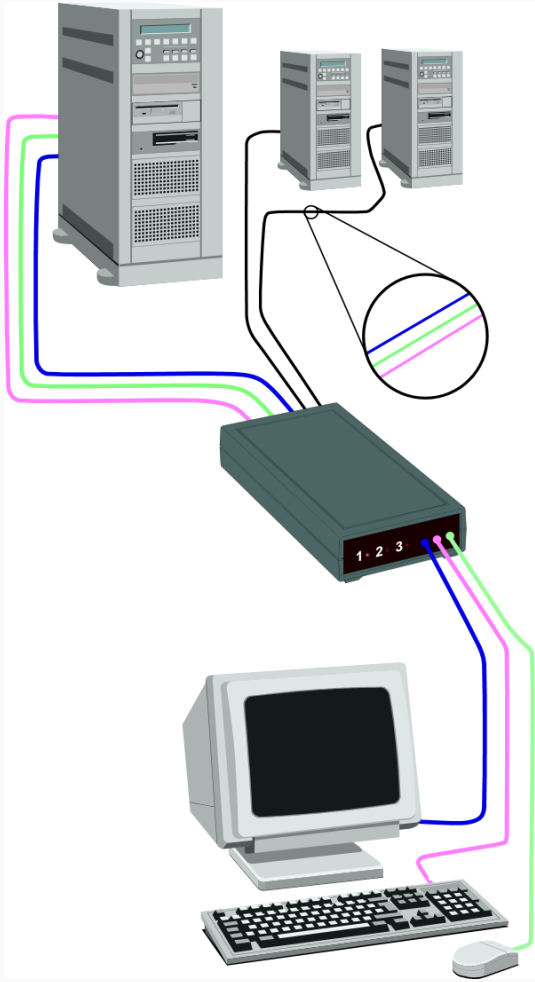
Sahasrar
Computing Facility
for
DST Funded
Research in Materials
Science

What is HPC? (p.35)

Infrastructure

Computing

- 3 labs for students $\sim$ 100 computers
- 2 research laboratories
- Self-maintained servers:
  Local cloud, web, mail, NAS, ...
- Large collection of open-source and special-purpose software
- Network storage, personal web space
- 24x7 access to premises
- 24x7 internet & WiFi (courtesy of SPPU)
- Moodle@CMS: For course management



Moodle@CMS – `http://apps.cms.unipune.ac.in/moodle/`

Infrastructure

Library

- $\sim$ 3000 books
- Magazines & journals
- Online resources
- Spacious reading hall

Building

- Currently, $\sim$ 10,000 sq.ft.
- Floor 1 construction in progress for School of Scientific Computing

Getting there ...

Research & Consultancy

8 Funded Research & Consultancy Projects $\sim$ Rs 10.65Cr (2011–)

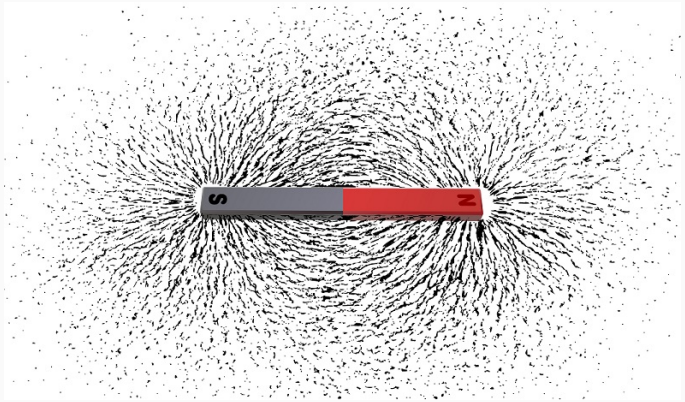
Defence: Weapons Ballistics
Industrial Modeling
Computational Materials Science
Computational/Systems Biology
Grid Computing

DST (Rs 9.19Cr)
DBT (Rs 1.1Cr)
DRDO (Rs 10L)
UGC (Rs 6L)
European Commission (EUR 39K)
SPPU + PennState (US$ 13K)
SPPU (Rs 2.75L)
Private Industry (Rs 50K)

Funding Details (p.37) | Research Groups (p.38)

Research/Consultancy Highlights

Predicting Target Accuracy Using M&S: Field Trials are Expensive (p.11)



Complex Magnetic Structures in Alloys: Important for Technology (p.39)

Statistical Science: From Genomes to Universe (p.40)

Materials for Energy Applications: Critical for Survival (p.41)

Research/Consultancy Highlight: Sukratu Barve

CFD Analysis of 120mm FSAPDS Tank Ammunition: ARDE–DRDO MBT Group, 2013–16. Project Cost: Rs 80,00,000

Understanding interior, intermediate, and exterior ballistics of tank ammunition.

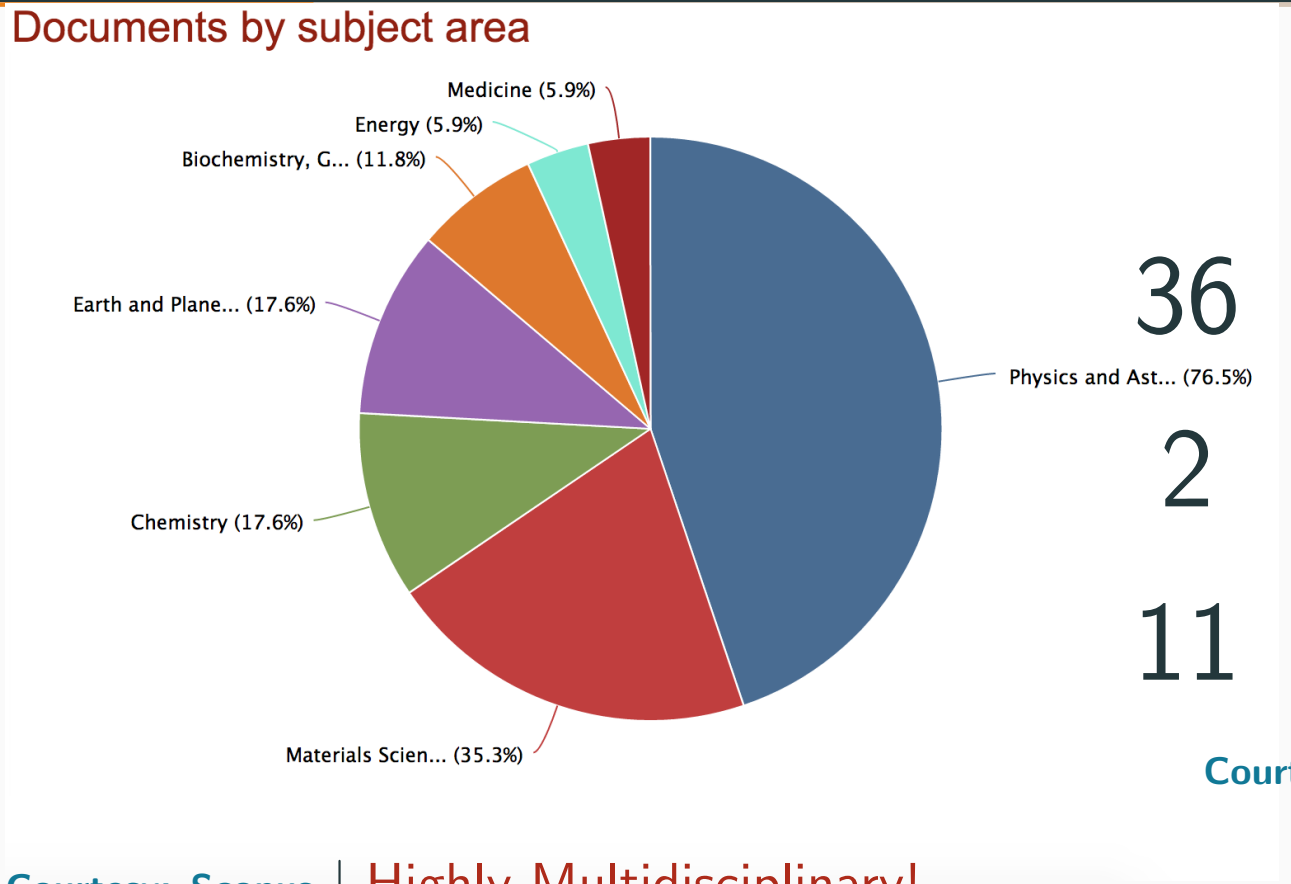
- Setting up mathematical models and carrying out simulations.
- Designing, implementing, testing, and delivering a customized open-source software package for the above.

Predicting target accuracy using M&S: Field trials are expensive!

Modeling the Action of a Thermact: Abhitech Energycon Ltd (Mumbai), 2010–11. Project Cost: Rs 50,000

Understanding how combustion-enhancing additives in coal-fired furnaces help maximize yield.

Research Publications 2011–



Courtesy: Scopus | Highly Multidisciplinary!

36 Journal Articles

2 Book Chapters

11 Conference Proceedings

Courtesy: research.unipune.ac.in

Impact factor range: 0.4 to 9.2*

All in reputed international peer-reviewed research journals

* Nucleic Acids Research 5yr IF: 8.647 | DOI: 10.1093/nar/gks1285

Individual Research Collaborations Involving CMS Faculty

Visualization based on co-author affiliations

Details (p.43)

Academic Programmes

Flagship Programme

- MTech Programme in Modeling & Simulation Details (p.44)

For Sponsored Students (Industry, Institutes)

- MTech Programme in Modeling & Simulation (Part Paper, Part Research)

http://cms.unipune.ernet.in/reports/pd-20160527/

Certificate Courses

- Fundamentals of Corporate Computing (Recently Approved)
- Linux Basics, LaTeX, etc.

PhD and MPhil

- CMS faculty are recognized guides for PhD/MPhil in Physics and Scientific Computing (Multidisciplinary!)

MTech Programme in Modeling & Simulation

One of its kind in India – A pioneering initiative

Very few similar broad-based programmes around the globe

Details (p.44)

http://cms.unipune.ernet.in/reports/pd-20160121/

MTech Programme in Modeling & Simulation

Applied mathematics + applied statistics + computing + M&S

2-Year, Post-BE/BTech
Core courses + choice-based credit courses + internship

Multidisciplinary, focused on methodologies
Relevant to academics *and* industry

Meticulous exposition of our philosophy of M&S,
pedagogy/didactics, and education in general

Course and learning management with Moodle@CMS

Details (p.44)

Curriculum Design

- Stakeholder involvement: industry experts, academicians, alumni
- Compliant with UGC's guidelines for choice-based credit system
- Delicate balance between
  - theoretical, applied, & hands-on
  - career possibilities: academic, corporate/industrial
  - fundamental knowledge & latest in technology
- Careful time-budgeting of student's work hours
- Addressing student weaknesses
  - self-study, learn-unlearn-relearn
  - time and stress management
  - out-of-box thinking
  - communication and presentation

Administrative Summary (p.45) | Curriculum Outline (p.46) | Implementation (p.47)
Enrichment Activities (p.48) | Enrollment & Performance (p.49) | Student Support (p.50)

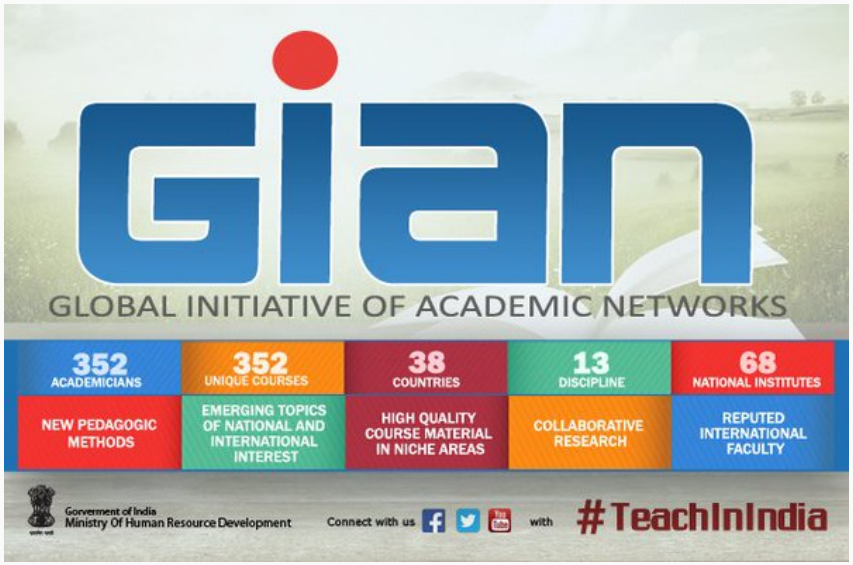
Learning Outcome

- **100%** students are employed within months of passing
- Recruitment via referred placements and project internship
- Equipped with fundamental knowledge + latest in computing technology, students choose both industry & academic careers
- Popular internship & career fields
  - Computational fluid dynamics (CFD)
  - Computer-assisted engineering (CAE)
  - Operations research (OR)
  - Data science and machine learning

Popular internship areas (p.20)

Representative placements (p.21)

Student Enrichment



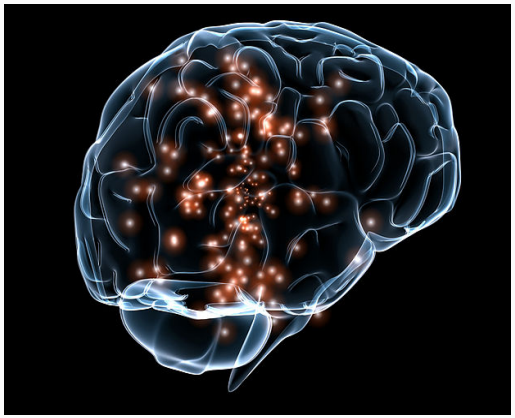
CMS was proud host to 2 GIAN courses (November 2016)

Functional Neuroimaging (Dr. Rebecca McNamee, US)

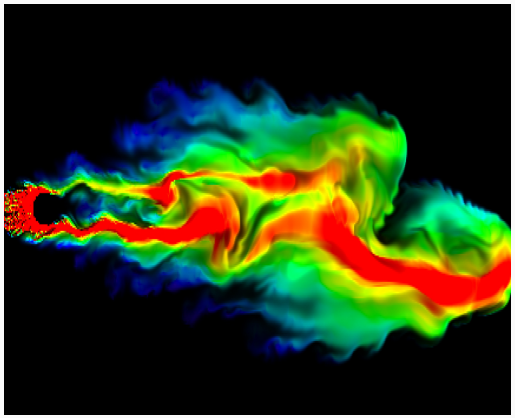
Fracture Mechanics (Prof. John Landes, US)

Other Enrichment Activities (p.48)

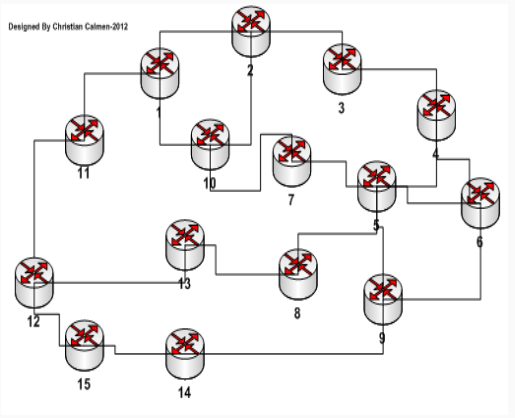
Popular Student Internship Areas



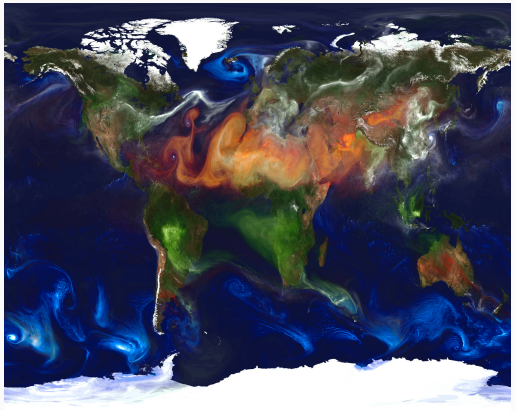
Machine Learning



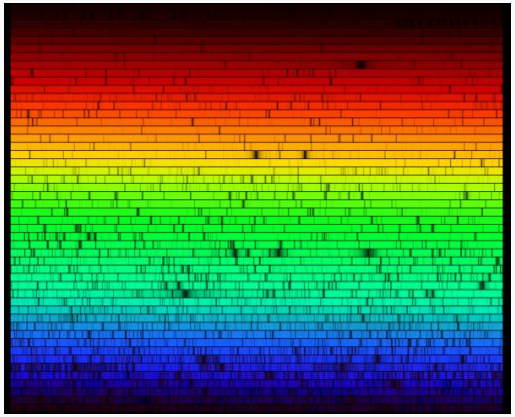
Computational fluid dynamics



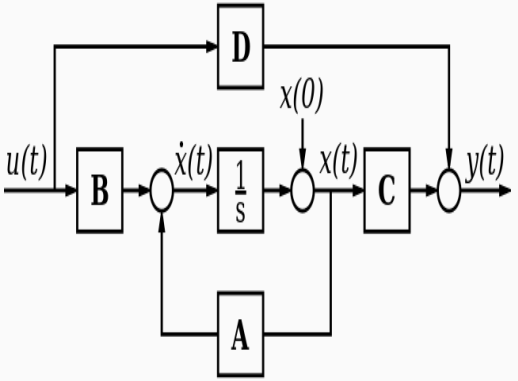
Operations Research



Atmospheric Modeling



Digital signal processing



Control Systems

Representative Placements: Industry & Academics

MPI, Germany

GMU, USA

INP Grenoble, France

Empa, Switzerland

KAUST, Saudi Arabia

HBCSE, Mumbai

IIT Bombay, Mumbai

IISER, Pune

Student Success Highlight

CMS student teams have ranked within top 5-10% in

international crowd-sourced data science competitions

Mentor: Prof. V.K. Jayaraman, Adjunct Emeritus Professor

. . . CMS has been running one of the best programs in modeling and simulation that I have ever come across. The vision, the comprehensive approach in both theoretical as well as applied aspects, the very careful nurturing of students, strong links with industry & high-quality research that is carried out by faculty [. . .] deserve all the encouragement & support that can be provided . . .

– Prof. N.V. Joshi (IISc) to Hon'ble Vice Chancellor, 2009

SWOC

Strengths

- Curricula: Rigorous, yet employment-friendly
- Team: Dynamic & dedicated, multidisciplinary to the hilt
- Uncompromising on academic values, yet supportive of weaker elements
- Driven to excel, despite the system

Weaknesses

- Programmes need to be publicized (aka "marketed")

SWOC

Opportunities

- Potential for diversification
- M&S: Relevant to industry & academics
- M&S: Relevant nationally & internationally

Challenges

- Funds, survival, stability
- Long-term faculty positions, critical faculty mass
- Lack of public-sector awareness about M&S, CMS, and MTech@CMS
- AICTE recognition: University-level effort under way
- Volatile national education policies: Not conducive to multidisciplinary programmes

Thank You

The Acid Test: What Students Say About CMS

Yes! I got very good salary hike while switching to new company, thanks to CMS.

Satadru Bera (2013-15). Senior Analyst in Vehicle Crash Simulation Field.

Yes, CMS experience helped . . . furthering my career.

Nitin Katakdound (2008-10). ICERTIS-Microsoft – Best Team Member Award.

. . . expertise in the R language, unix scripting, high-performance computing, and mathematical modeling and simulation, which I learnt at CMS only.

Sagar Kashid (2008-10). Support Scientist, Climate Modeling Group, CDAC, Pune.

MTech . . . a perfect blend of theoretical knowledge and applied engineering.

Jitender Yadav (2008-10). Avionics Systems Engineer at Honeywell International.

The curriculum is one of a kind . . . culture at CMS is very simply "for the students"

Anirudh Jonnalagadda (2014-16). Pursuing PhD at IIT-B.

From biology background . . . I could shift easily to computational biology due to CMS

Rashmi Kulkarni (2008-10). Completed PhD at IISER, Pune.

My tenure at CMS . . . opened up many interesting possibilities . . .

Sarvesh Nikumbh (2010-12). Pursuing PhD at MPI-INF, Germany.

Additional Information: Vision

Vision

Established in 2003 through generous seed funding (UGC/UPE), to

- promote, support, and facilitate academics and research in mathematical modeling and computational simulation;
- promote use of computation as the third scientific methodology;
- promote highly multidisciplinary approaches that transcend (artificial) boundaries separating traditional knowledge domains;
- promote a problem-centric outlook for real-life scientific and technological problems;
- nurture strong expertise in state-of-the-art computing technologies;
- nurture computing culture on the University campus.

Back (p.4)

Additional Information: Faculty & Staff

Faculty & Staff

Director

- Anjali Kshirsagar, PhD

Associate Professors

- Mihir Arjunwadkar, PhD

Assistant Professors

- Sukratu Barve, PhD
- Bhalchandra Gore, PhD
- Bhalchandra Pujari, PhD (UGC)

Distinguished/Adjunct Professors

- Dilip Kanhere, PhD
  Distinguished Professor
- V.K. Jayaraman, PhD
  Adjunct Professor

Post-Doctoral Researchers

- Vikas Kashid, PhD
- Narasimham, PhD
- Kavita Gangal, PhD
- Deepak Bankar, PhD

Academic/Placement Coordinator

- Shilpa Jain, PhD

Administrative/Technical

- Mrunalini Dharmadhikari
- Vaibhav Rajkuwar
- Vaneeta Thokal
- Gajanan Rakhunde
- Satish Waman

Back (p.5)

Awards & Recognitions

Bhalchandra Pujari

- UGC Faculty Recharge Programme, 2013–

Sukratu Barve

- Best Poster Prize: International Conference on Gravitation & Cosmology, 2011

Mihir Arjunwadkar

- Editorial Board of the *Resonance* Magazine

Faculty

- Referees to Reputed International Peer-Reviewed Journals
- Routinely Invited as Resource Persons

Anjali Kshirsagar

- Prin. V.K. Joag Award (2011): Excellence in Teaching and Research
- Senior Group Associate of ICTP Trieste, Italy (2002–14)
- Member and Chartered Physicist, Institute of Physics, UK

Dilip Kanhere

- Fellow of the Indian Academy of Science, Bangalore

Back (p.5)

Visiting Faculty

- V.V.N. Kishore
  PhD Chemical Engineering
- Abhijat Vichare
  PhD Physics
- Pratip Shil
  PhD Physics
- Sanjay Kadam
  PhD Mathematics
- D. Gadkari
  PhD Geography
- Sheelan Chowdhury
  PhD Physics
- Akanksha Kashikar
  PhD Statistics
- Mrs. Manjusha Joshi
  MPhil Mathematics
- Sunil Gokhale
  PhD Physics
- Kshama Rahirkar
  MSc Statistics
- Padma Pingle
  MSc Mathematics
- Mohan Kale
  PhD Statistics
- Leelavati Naralikar
  PhD Computer Science

... and many more ...

Back (p.5)

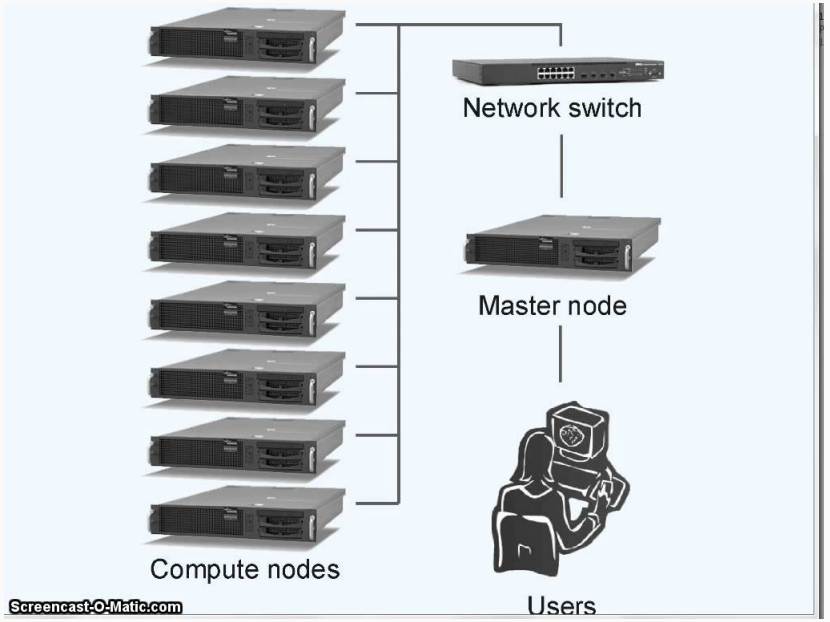
Additional Information: Infrastructure

High-Performance Computing Clusters

Connecting together several small computing units through fast interconnects, HPC makes it possible to solve large & daunting mathematical and computational tasks.

HPC is used in virtually all domains of advance research; e.g., materials science, atmospheric science, astrophysics, chemistry, computer aided engineering, etc.

Sahasrar@CMS has 1000+ computing units (cores) on 50 nodes connected together to performs 50 $\times 10^{12}$ mathematical operations in just one second!



Back (p.6)

Additional Information: Research

Research Funding 2011– 8 Projects ∼ Rs 10.65Cr

Bhalchandra Pujari

- Start-Up Grant (UGC, 2014) — Rs 6La
- Materials Under Pressure (SPPU, 2016-18) — Rs 2.7La
- One-Way Propagation of Heat (SPPU-PennState, 2016-17) — US$ 13K

Sukratu Barve

- Professional Services for CFD Analysis (IDST/DRDO, 2014-16) — Rs 10La
- Modeling the Action of a Thermact (Private Industry, 2010-11) — Rs 50K

Mihir Arjunwadkar

- Systems Biology of Global Regulatory Networks (DBT, 2009-12) — Rs 1.1Cr

Anjali Kshirsagar

- Computational Studies on Novel Materials and Nanoscale Transport (DST NanoMission, 2012-16) — Rs 9Cr
- Nanostructures with Novel Functionalities (DST, 2012-15) — Rs 18.7La

Dilip Kanhere

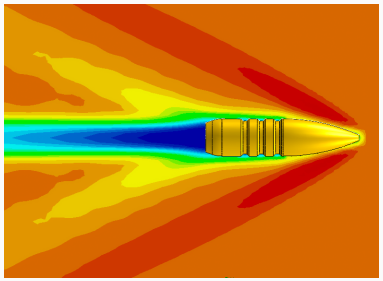
- EU-India Grid (European Commission, 2009-11) — EUR 39K

Back (p.9)

Research Groups

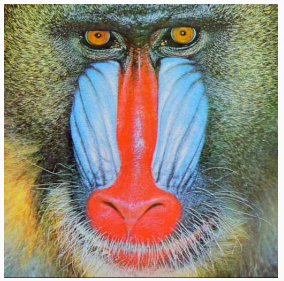
Computational
Materials
Atomistic Modeling

Bhalchandra Pujari
Anjali Kshirsagar
Dilip G. Kanhere



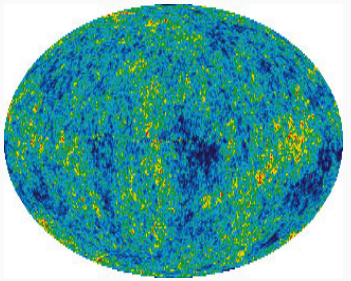
Computational
Fluid Dynamics
Weapons Ballistics
Industrial Mathematics

Sukratu Barve



Digital Signal & Image
Processing

Bhalchandra Gore



Statistical Science
Astrostatistics
Data Science
Machine Learning

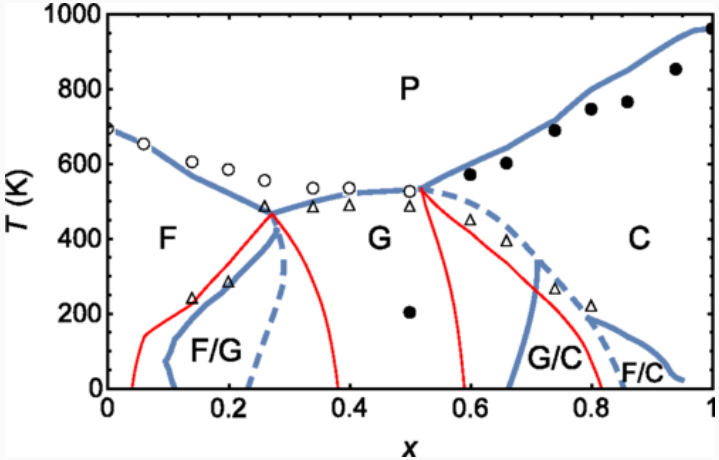
Mihir Arjunwadkar
V.K. Jayaraman

Back (p.9)

New Method for Magnetic Behaviour of Alloys

- Development of novel method to determine the complex magnetic structures in Random Alloys
- Purely ab-intio technique
- Replication of magnetic phase diagram
- Prediction of new magnetic phase of Fe-MnPt alloy, undetected so far

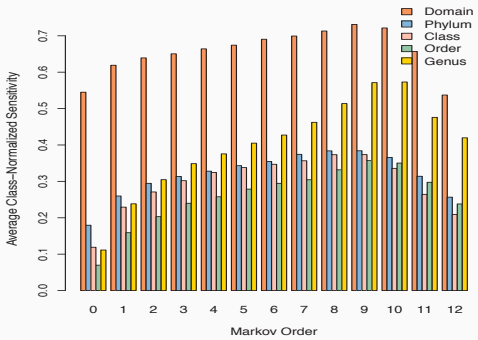
Published in *Physical Review Letters*



Back (p.10)

Research Highlight: Mihir Arjunwadkar

Statistical Science: Understanding the World Through Data

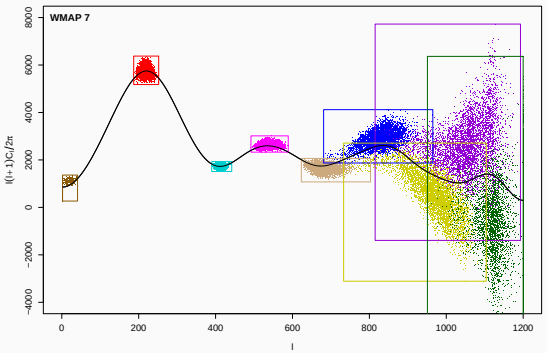


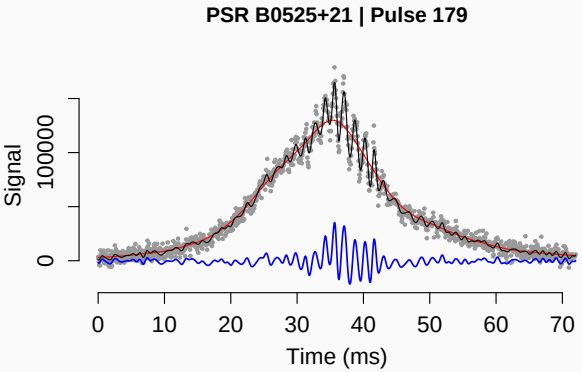
One Size Does Not Fit All: Order Selection for Markov Models of Genomic Sequences

Nucl Acids Res (2012) 41(3) 1416-1424 (DOI:10.1093/nar/gks1285)

Cosmic Microwave Background Power Spectrum: Nonparametric Reconstruction

The Astrophysical Journal (2012) 745(2) 745-114 (DOI:10.1088/0004-637X/745/2/114)
Phys Rev D (2014) 89 023509 (DOI:10.1103/PhysRevD.89.023509)
Journal of Cosmology and Astroparticle Physics (2015) (DOI:10.1088/1475-7516/2015/02/007)





Pulsars and Neutron Stars, GMRT and SKA

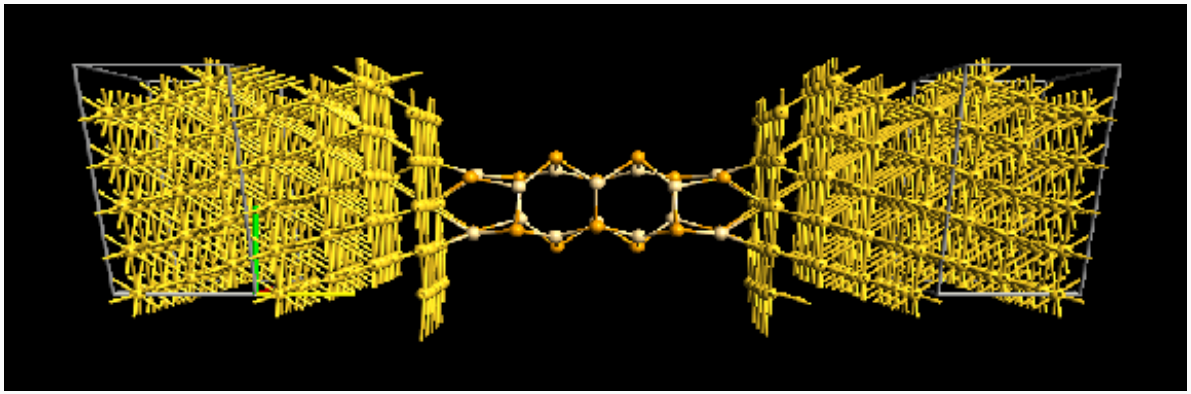
The Astrophysical Journal (2015) 806(2) 226 (DOI:10.1088/0004-637X/806/2/236)
MNRAS (2016) 460(3) 3063-3075 (DOI:10.1093/mnras/stw1186)
J Astrophysics & Astronomy (2016) 37(4) 28 (DOI:10.1007/s12036-016-9410-0)

Back (p.10)

Materials for Energy Applications

- II-VI Semiconductor alloy or core-shell quantum dots for solar cell applications
- Two-dimensional materials for hydrogen and oxygen evolution reactions for water splitting
- Combination of metal-semiconductor and semiconductor-semiconductor surfaces for Schottkey barrier and excitonic solar cell

Structure prediction with M&S!

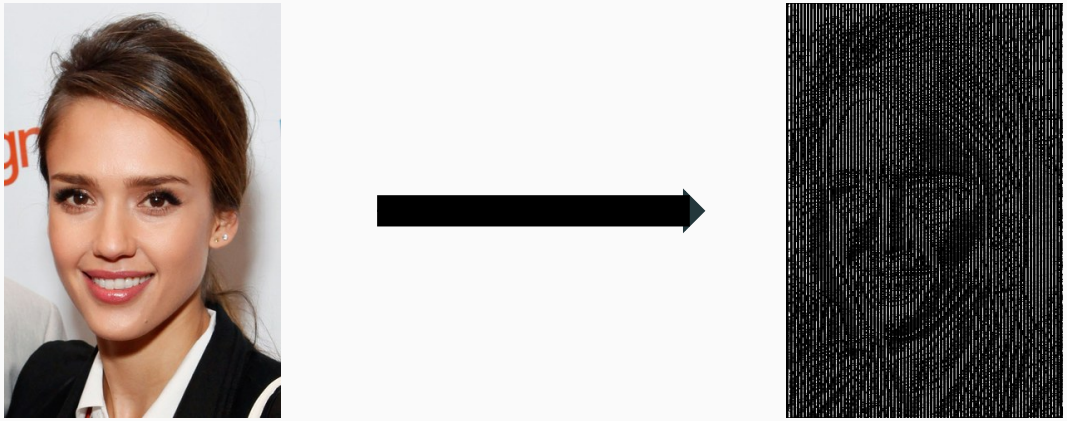


Connecting nanodevices

Back (p.10)

Digital Processing of Signals & Images

- Automated identification of **voice**, **gender**, **features**, **handwriting** for use in cognitive detection systems



- speaker identification for the captured voice recording
- to measure security strength cryptographic keys (in terms of time for breaking) – in collaboration with Dr. Smita Bedekar, ISSC-SPPU.

Back (p.10)

Individual Research Collaborations Involving CMS Faculty

Co-Author Affiliations

NCRA-TIFR, India
IUCAA, India
IISER-Pune, India
IMSc, India
SPPU, India
ICTP, Italy
University of Vermont, USA
University of South Florida, USA
Korea Astronomy and Space Science Institute, South Korea
University of Basel, Switzerland
Uppsala University, Sweden
Max-Planck-Institut für Radioastronomie, Germany
University of West Virginia, USA
National Radio Astronomy Observatory, USA
Jet Propulsion Laboratory, USA
Penn State University, USA
University of Nebraska-Lincoln, USA

Back (p.13)

Additional Information: Academic Programmes

MTech in Modeling and Simulation

Administrative Summary

Programme Level	Post-Graduate
Sanctioned Intake	30
Entry Qualification	BE or BTech
Selection	Through Entrance Test
Duration	4 Semesters
Total Credits	100 (25 credits/semester)
Credit Break-Up	58 Core, 17 Choice-Based, 25 Internship
Internship	1 Semester (25 credits)
Examination	Semester Pattern
Assessment	Continuous
Commencement	2008
Revisions	2012, 2016

Back (p.17)

MTech in Modeling and Simulation

Semester 1

Core credits: 25, choice-based/elective credits: 0

Code (Section)	Course Name	Credits
C101 (2.2)	Real Analysis and Calculus	2
C102 (2.3)	Vector Analysis	2
C103 (2.4)	Linear Algebra	2
C104 (2.5)	Ordinary Differential Equations	2
C105 (2.6)	Partial Differential Equations	3
C106 (2.7)	Probability Theory	3
C107 (2.8)	Computing with `R`	1
C108 (2.9)	Computing with `MATLAB/Scilab`	1
C109 (2.10)	Computing with `C`	2
C110 (2.11)	Algorithms	2
C111 (2.12)	M&S Hands-On 1	5

Semester 2

Core credits: 18, choice-based/elective credits: 7

Code (Section)	Course Name	Credits
C201 (2.13)	Complex Analysis	2
C202 (2.14)	Transforms	2
C203 (2.15)	Difference Equations	2
C204 (2.16)	Numerical Computing 1	2
C205 (2.17)	Optimization 1: Deterministic	2
C206 (2.18)	Statistical Inference	3
C207 (2.19)	M&S Hands-On 2	5

Semester 3

Core credits: 15, choice-based/elective credits: 10

Code (Section)	Course Name	Credits
C301 (2.20)	Numerical Computing 2	2
C302 (2.21)	Optimization 2: Stochastic	3
C303 (2.22)	Stochastic Simulation	3
C304 (2.23)	M&S Overview	4
C305 (2.24)	M&S Apprenticeship	3

Semester 4

Core credits: 25, choice-based/elective credits: 0

Code (Section)	Course Name	Credits
C401 (2.25)	Internship	25

Curriculum Outline:
2016 Revision

http://cms.unipune.ernet.in/reports/pd-20160121/

Back (p.17)

Programme Implementation

- Highly accessible teachers & mentors
- Prudent use of Moodle@CMS, a reputed course management system
- Personalized mentoring and monitoring of students
- Friendly learning and work environment
- 24x7 access to premises, labs, learning resources, internet
- Multiple assessment mechanisms, from conventional to online
- Multiple feedback mechanisms, including an online portal
- Emphasis on hands-on work and internship

Moodle@CMS – `http://apps.cms.unipune.ac.in/moodle/`

Back (p.17)

Academic Enrichment Activities

GIAN Courses 2016

- Functional Neuroimaging (Dr. Rebecca McNamee, US)
- Fracture Mechanics (Prof. John Landes, US)

Theme-Based Workshops

- M&S in the Public Sphere (2015)
- M&S in the Defence Sector (2017)

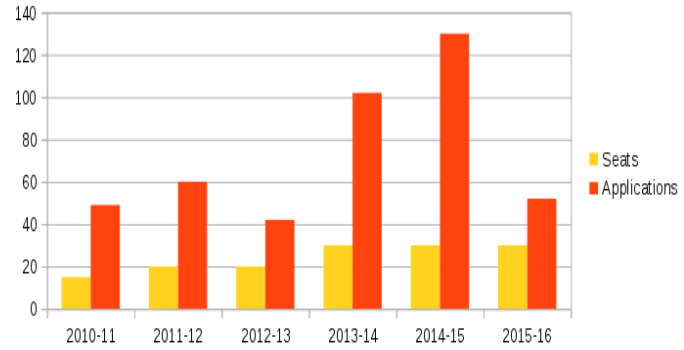
M&S Colloquia, Research Seminars

- $\sim$ 15 during 2011-16

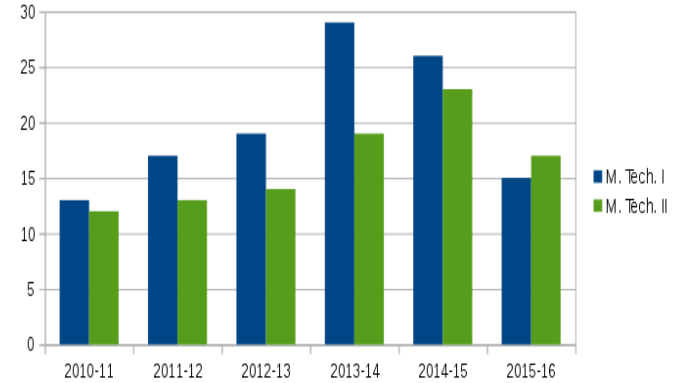
Back (p.17)

Student Enrollment and Performance Statistics

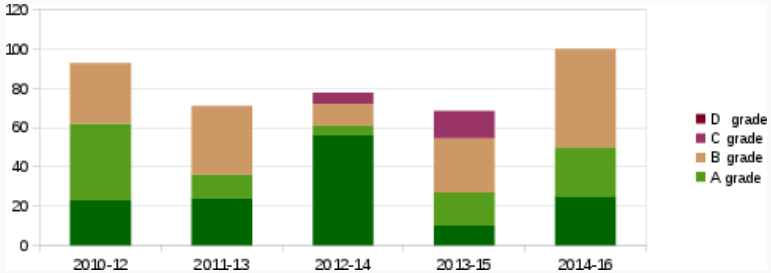
Entrance exam applications



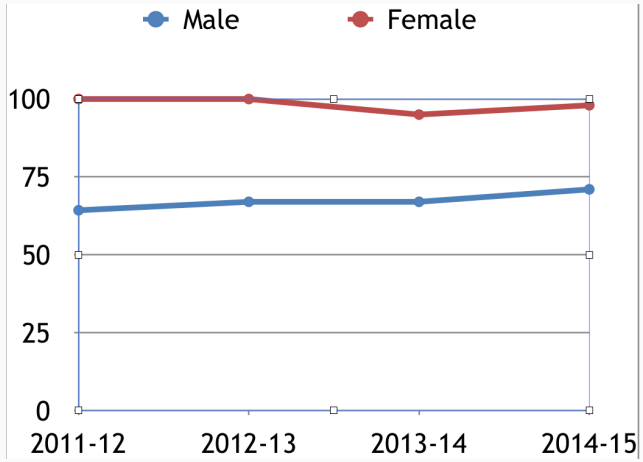
Admissions



Passing percentage



Female students perform better!



Back (p.17)

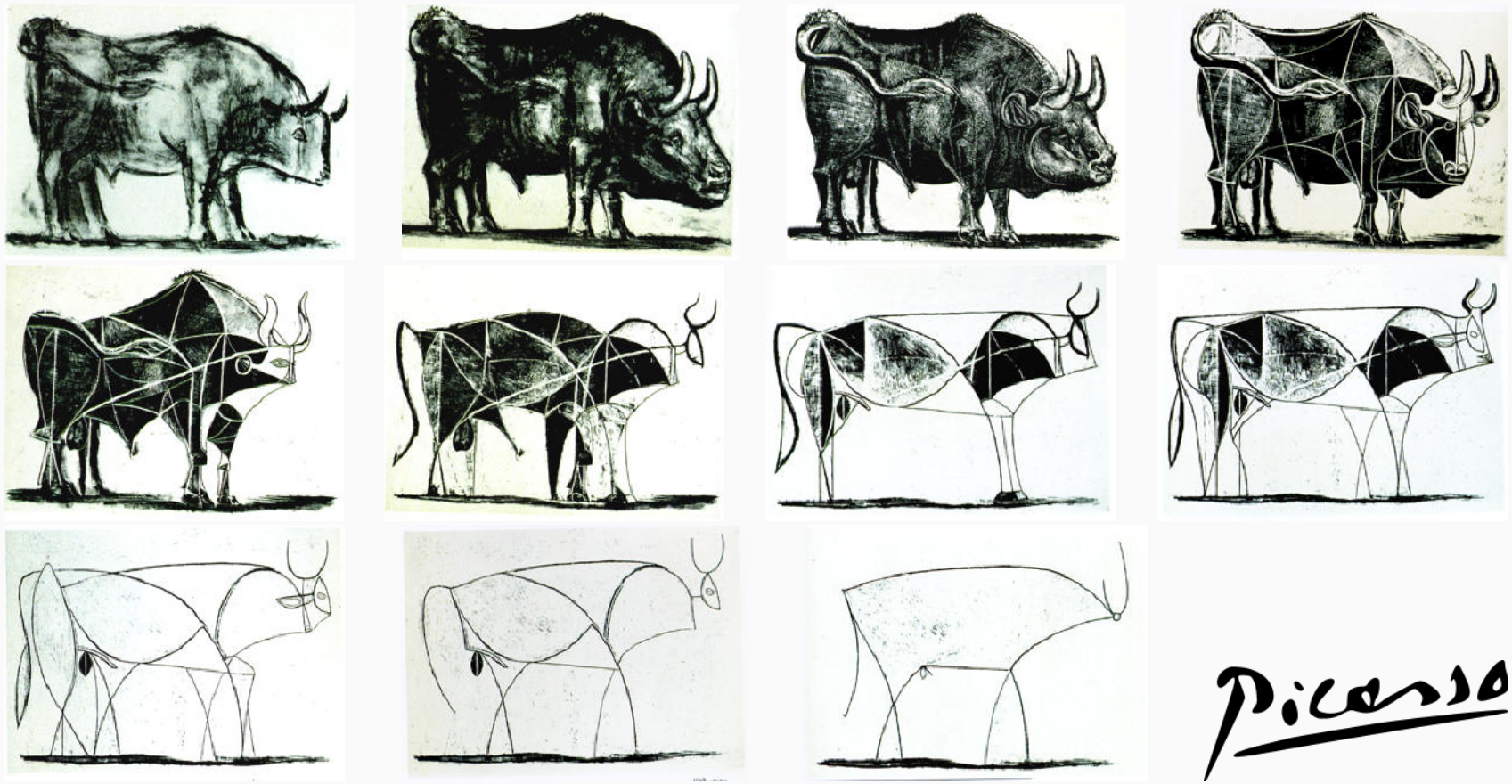
Student Support

- Highly accessible faculty members
- Student-centric learning and work environment
- Individualized student mentoring
- Friendly culture conducive to education
- Support for scholarships offered by SP Pune University
- Dedicated academic/placement coordinator
- Facilitating placements: Liaison between recruiters and students

Back (p.17)

Additional Information:
A Cartoon Guide to M&S

The Spirit of Scientific/Mathematical Modeling

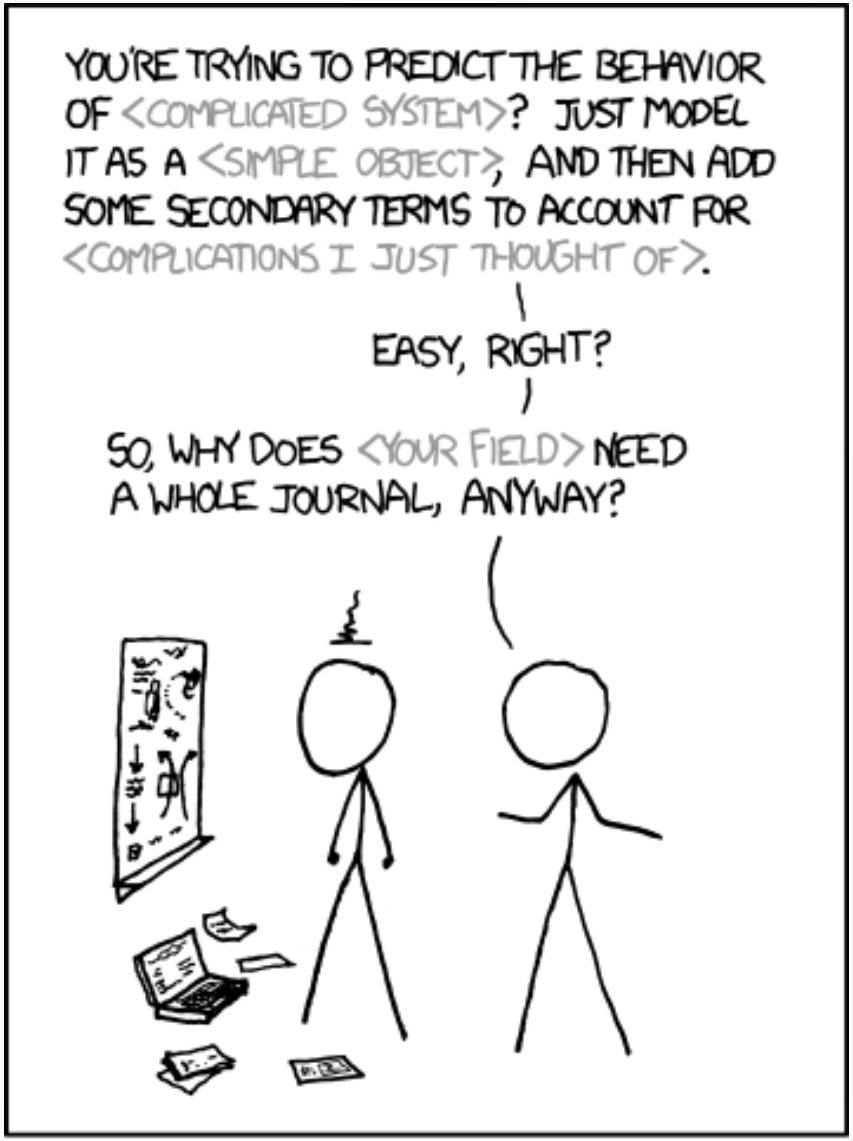


Back (p.4)

The Spirit of Scientific/Mathematical Modeling

- Abstraction: Keep only the essential in the context of the question being investigated
- Express relationships in the language of mathematics; this is the model
- Explore model through simulation/computation
- Validate model against reality; modify it if required
- ...

Back (p.4)



The Spirit of Scientific/Mathematical Modeling

Principle of Parsimony

aka

Occam's Razor

Back (p.4)

The Spirit of Scientific/Mathematical Modeling

...

The fact that the polynomial is an approximation does not necessarily detract from its usefulness because all models are approximations. Essentially,

all models are wrong, but some are useful.

However, the approximate nature of the model must always be borne in mind.

...

George E. P. Box

Empirical Model-Building and Response Surfaces (1987, p 424)

Back (p.4)

The Spirit of Scientific/Mathematical Modeling

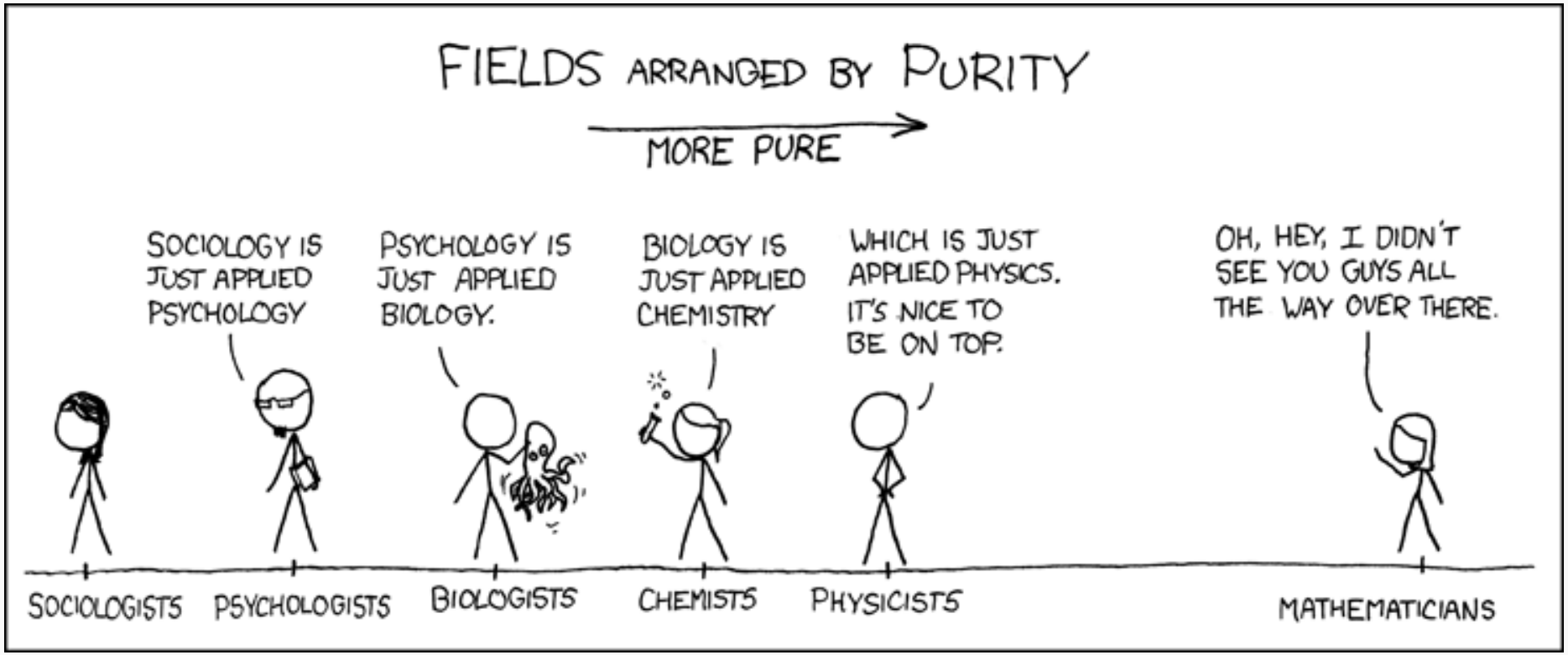
all models are right, most are useless.

Thaddeus Tarpey

`http://works.bepress.com/thaddeus_tarpey/44/`

Back (p.4)

Over-compartmentalization of knowledge?



mathematical models + computation/simulation

cut across

knowledge domains and disciplines

Back (p.4)