IISc

Department of Computational and Data Sciences

Division of Interdisciplinary Sciences, Indian Institute of Science, Bengaluru

Welcome to CDS

CDS

Department of Computational and Data Sciences

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About IISc

- India's premier research and teaching institute of higher education
- Consistently ranks among the top 10 small universities globally
- Renowned for its focus on research excellence, academic freedom and attracting high quality of students (top 1% of applicants) and faculty

About CDS

- An interdisciplinary engineering department at IISc spanning the research areas of Computational Science and Engineering, and Computer and Data Systems
- Besides pursuing cutting edge research, CDS faculty leads several national and international initiatives, and provide industrial consultancy and research services

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Research Groups/Labs

Computational Science and Engineering

1. Medical Imaging Group (MIG): *Phaneendra Yalavarthy*
The research group works on developing computational methods/models in medical imaging. The recent focus has been toward deep learning methods for medical image reconstruction and analysis.

2. Biomolecular Computation Laboratory: *Debnath Pal*
The focus of Biomolecular Computation Lab is to understand biological function at multiple scales. Towards this goal we work at molecular level and pathway level and develop methods and algorithms to understand biochemical function better. The scope of work spans the areas of genomics, proteomics and metabolomics. We also work on bio-molecules to understand sequence, structure function relationships, their interactions and dynamics.

3. Structural Biology & Bio-Computing Lab: *K. Sekar*
The research group focuses on solving three-dimensional crystal structures of protein molecules using X-ray crystallography and molecular dynamics simulations. Further, we are also interested in data mining of protein sequences and structures.

4. Computational Mathematics Group: *Sashikumaar Ganesan*
The research group focuses on the development and advancement of robust numerical (finite element) methods and solver for solving partial differential equations (PDEs) that describe incompressible fluid flows and species concentration and/or energy in complex systems. The group also works on implementing efficient parallel algorithms for high-performance computing.

Research Groups

Computational Science and Engineering

5. Scientific Computation Lab (SCL): *Soumyendu Raha*
Control and Optimization of Constrained Dynamical Systems, Stochastic and Deterministic Differential-algebraic equation systems, Mathematical Libraries, VLSI CAD applications.

6. Computational & Statistical Physics Lab: *Murugesan Venkatapathi*
This group is interested in certain areas of physics, or mathematical analysis, or scientific algorithms. Examples of our recent results include a theory of strong-coupling of emitters with dissipating matter, computational method for quantum N-body problems in emission, analysis of polynomial recurrence relations and fast computing methods for eigenvalue problems, methods of estimation to substitute Markov-Chain-Monte-Carlo (MCMC) sampling, and error estimators for linear solvers.

7. QUEST (Quantifying Uncertainty in Engineering, Science and Technology) Lab: *Deepak Subramani*
The goal of our research is to build holistic science-based data-driven computational solutions to complex engineering and environmental problems. Example applications include climate change, cyclone predictions, coastal hazard management, and optimal vehicle routing. We are interested in numerical solution of stochastic partial differential equations, uncertainty quantification, Bayesian and deep learning of dynamical systems, fluid dynamics of the atmosphere and oceans, and path planning of autonomous vehicles in dynamic environments.

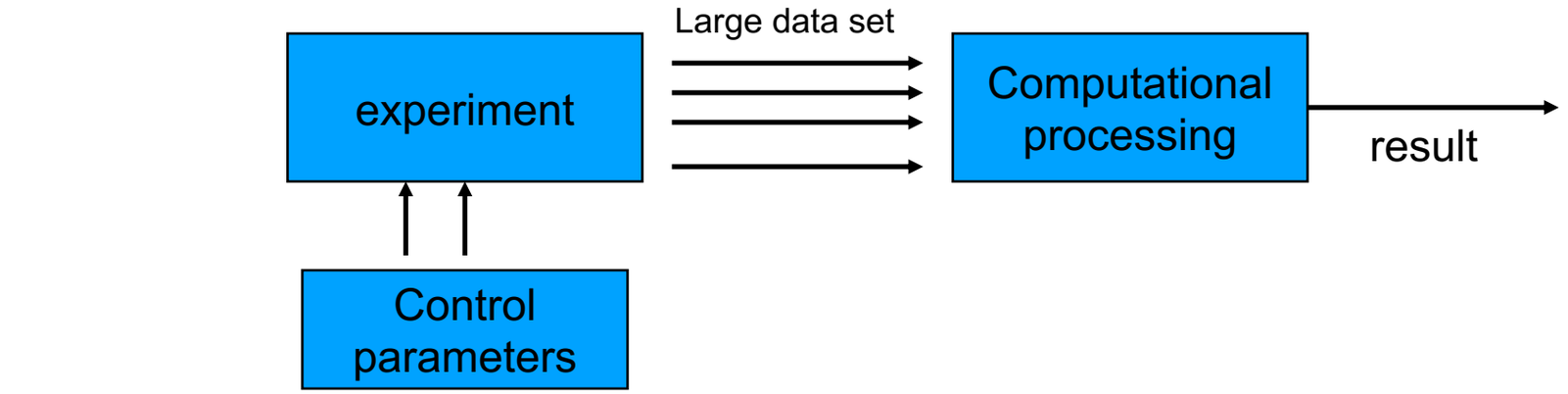
8. Computational Flow Physics Lab: *Konduri Aditya*
The research group focuses on the simulation and analysis of multi-scale multi-physics fluid flow problems that leverage high performance computing (HPC) platforms. Specifically, the work would involve development of HPC centric numerical methods and algorithms for solving partial differential equations, application of machine learning methods to analyze and model data generated from simulations, and investigation of turbulent flow problems that arise in combustion systems, high-speed aerodynamics and environmental flows.

Private scholarships/Awards

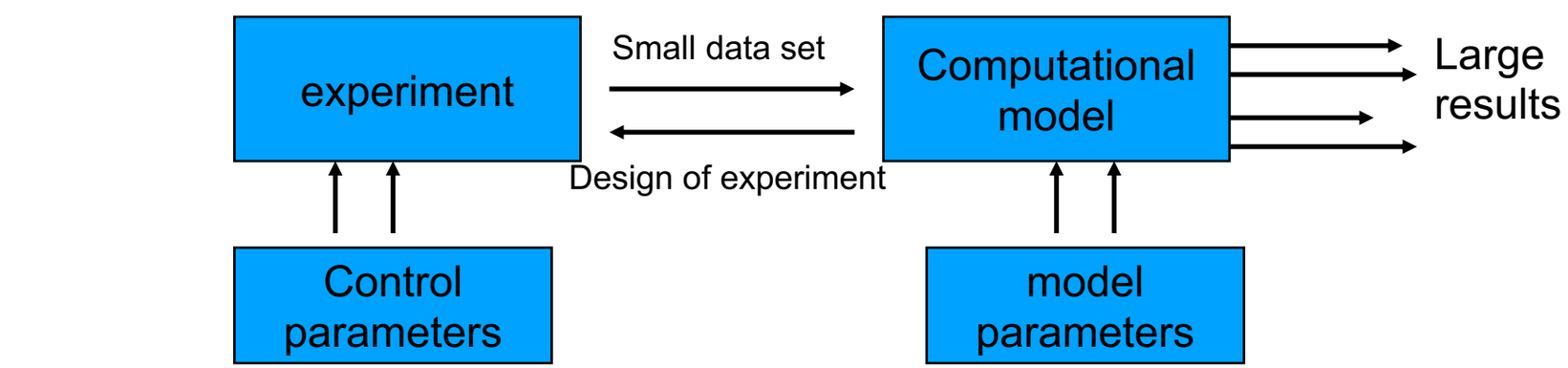
- Narayana Nethrayala Research Award:1
- Microsoft Data Science Fellowships for M.Tech. (Research): 2
- Intuit M.Tech. (Research) Fellowship:1
- Cargill M.Tech. Fellowships: 2
- Target India M.Tech. Fellowship:1
- TESCO Technology M.Tech. Fellowship:1
- GE Healthcare M.Tech. Fellowship: 1
- Ericsson M.Tech. Fellowships: 2
- ...

Computational & Data Sciences

Data Problem



Modeling Problem



Numerics example 1

$$\begin{pmatrix} 1 & 1000 \\ 0 & 1 \end{pmatrix}$$

Eigenvalues: 1, 1

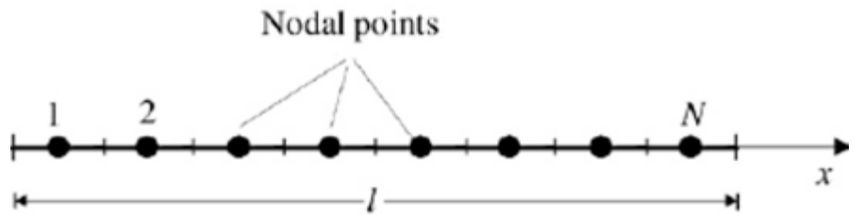
$$\begin{pmatrix} 1 & 1000 \\ 0.001 & 1 \end{pmatrix}$$

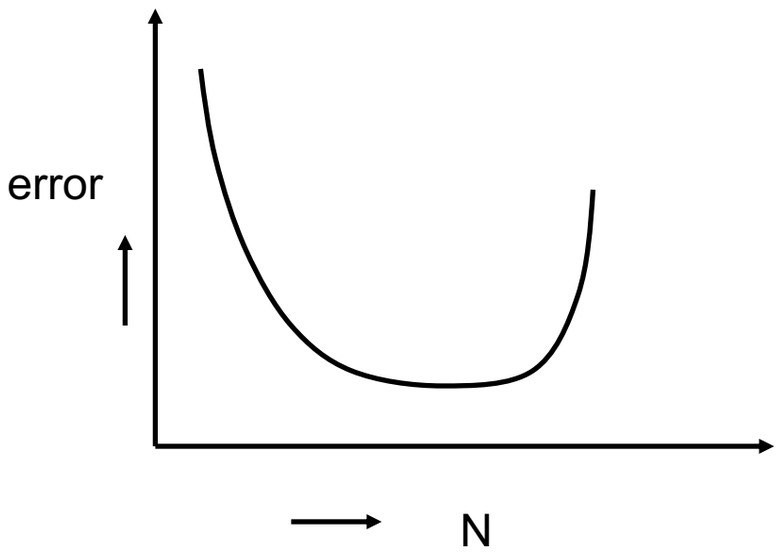
Eigenvalues: 0, 2

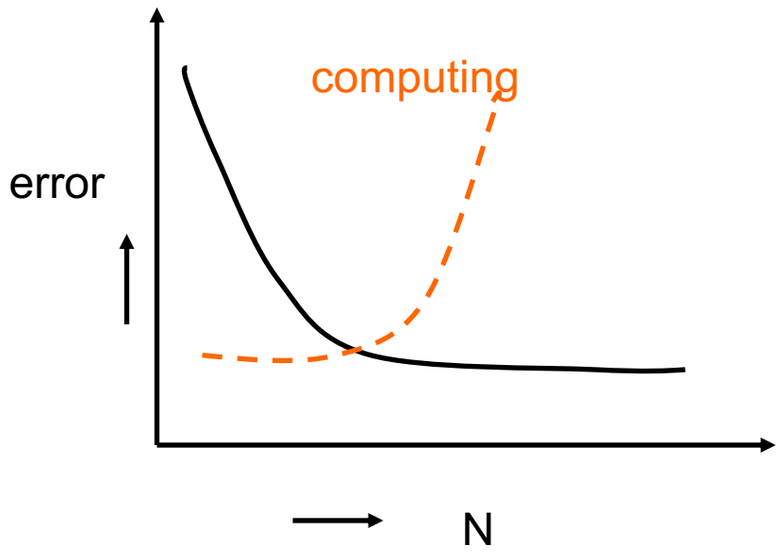
Increase in computational power due to computational methods/algorithms has also scaled like Moore's law on average !! Just that it is not as smooth and predictable.

Numerics example 2

Peril of naive discretization







CDS Courses

- Numerical Methods
- Numerical Linear Algebra
- Numerical Solutions of Differential Equations
- Modeling and Simulation
- High Performance Computing
- Data Structures and Programming
- Data Assimilation to Dynamical Systems
- Finite Elements: Theory and Algorithms
- Numerical Optimization

Areas & Examples

- Complex experiments at the frontiers of knowledge
- All engineering and chemical, biological, material sciences
- Cyber-physical systems
- Examples: tsunami warnings, large hadron collider, gravitational wave observations, drug discovery, medical imaging and diagnosis/prognosis