COMPUTATIONAL SCIENCE
AND SCIENTIFIC COMPUTING

INTRODUCTION & OBJECTIVES

The Strategic Research Programme (SRP) on Computational Science and Scientific Computing (CSSC) positions itself as a focal point for HPC-related activities. It strives to spearhead the development and application of advanced computational techniques involving HPC architectures and sophisticated software tools for research dealing with complex interdisciplinary engineering problems. It also aims to spearhead the integration of sophisticated mathematical techniques with engineering theory and advanced computer technology.

Centre for Advanced Numerical Engineering Simulations (CANES) and Nanyang Centre for Supercomputing and Visualisation (NCSV) are the two leading research centres that support this CSSC SRP. With CANES's core strength in HPC applied to interdisciplinary engineering problems, scientists and engineers are able to overcome the limitations associated with empiricism and improve the results and productivity of their R & D efforts. On the other hand, NCSV is a cutting-edge R&D centre that boasts state-of-the-art HPC and advanced data management technologies. Combining these supercomputing capabilities with advanced visualisation technologies, NCSV is the place NTU researchers turn to for extracting valuable insights through analysis of critical data.

RESEARCH CAPABILITIES

The SRP is well supported by our leading-edge high performance computing facilities. The main server farm consists of a SGI Origin 2000, a SGI Origin 3400 and a SUN Fire 15K compute server. Each possessing 32 processors with scalable configuration, the three servers are capable of crunching data and numerical calculations at blazing speeds. Currently the Origin 2000 is capable of doing calculations at 16 Giga-FLOPS, the Origin 3400 at 25.6 Giga-FLOPS and the SUN Fire 15K at 57.6 Giga-FLOPS. The facility is further augmented with a Storage Area Network of at least 2 Terabyte and increasing.

The server farm also consists of one 8 processors Sun Fire 4800, two dual processors E280R server, one 8 processors V880 server, two 4 processors V880 server, and twenty Unix graphical workstations. All these come together to provide researchers with a reliable and pervasive access to the compute and storage facilities. On top of that, an SGI Onyx 3 server equipped with one graphical brick drives a reality centre which greatly enhances our centre’s visualization capabilities.

In the pursuit of research excellence, the SRP has close collaborations with internationally renowned institutions such as the Massachusetts Institute of Technology, University of Queensland, University of Southern California, University of Toronto and Tsinghua University.
RESEARCH AREAS

This SRP focuses on ten main research areas covering Grid Computing; Computational Biomedical Engineering; Computational Fluid Dynamics; Multi-disciplinary Design Optimisation; Modeling of Micro-Electro-Mechanical Systems; Materials Modeling; Design, Integrity, Reliability and Failure Modeling; Meshless Methodology Development and Application; Computational Nanoscience – Multiscale Simulation; and Bio-Computing.

Grid Computing

A “Grid” is a software infrastructure that provides a flexible, secure, coordinated resource sharing among dynamic collection of virtual organizations. Using the Grid middleware, users are presented with a single virtual access to the campus supercomputers. With Grid Computing, the supercomputing facilities and high capacity storage systems installed in the various research centres and laboratories throughout the University can be fully exploited. Users can optimize productivity and focus on design and development of their research rather than hunting for resources. Just as the Web changes the way we communicate with each other, the Grid will change the way we access to the computation and storage resources.

To enable a practical Grid Computing, there are issues to be addressed:
- Global Resource Management
- Job Scheduling and Re-scheduling
- System Management
- Data Management
- Information Services
- Security
- Development Environment and Tools
Computational Biomedical Engineering (CBME)

The CBME program is aimed at constructing multi-physics mathematical models used in estimating diagnostic indices for various human organs. State-of-the-art computational methods from various engineering disciplines, medical imaging technologies and high performance computing are utilized. Medical practitioners will have more rational basis for making medical diagnosis, by comparing diagnostic indices of normal and diseased patients. It can play a significant role in the formulation of clinical tests. The tests will investigate the normal and pathological characteristics of physiological systems being studied, through exploring the response of organ systems to drug regimes and other interventions, and via examining the design and analysis of prostheses and organ-assisted systems. The goal of CBME is to collaborate with leading medical practitioners to further develop and advance the use of HPC in medical diagnosis, in the area of prostheses and organ-assist devices design, and pre-surgical simulations.

Computational Fluid Dynamics (CFD)

The CFD program is concerned with the development and application of numerical methods in solving the equations of fluid motion. It deals with the simulation of both compressible and incompressible flows. Typical activities include structured and unstructured grid generation, flow algorithm development for Compressible and Incompressible Navier-Stokes Equations based on finite difference, finite volume and finite element methods, Turbulence Modeling, Graphical Post-processing, and deploying High Performance Computing facilities.

Multi-disciplinary Design Optimisation (MDO)

The program in Multidisciplinary Design Optimization (MDO) is primarily aimed at combining state-of-the-art computational tools in various specialized engineering disciplines such as computational fluid mechanics, computational structural mechanics and computational electromagnetic. This is carried out with conventional optimization methods such as gradient-based search methods and with non-conventional optimization methods such as simulated annealing, genetic algorithms, mixed-integer programming, game theories and so on to bear on complex engineering design problems. MDO technologies help engineers to determine global optimum design solutions to engineering problems involving multi-objective functions and constraints, which result from multi-physics interactions.

Modeling of Micro-Electro-Mechanical Systems (MEMS)

During the last decade, MEMS technology has grown immensely and encompasses most technical disciplines with wide-ranging applications. Some of the modeling activities being investigated currently are in the areas of numerical simulation of micro-flow in micro devices which focuses on the application of Computational Fluid Dynamics (CFD) methodology, Rarefied gas theory, Monte Carlo methods and first and second order models with slip wall boundary conditions. Applications include micro-channel flow, micro (squeeze film) damping, free surface micro-jet, flow over micro-steps, and complex micro-fluidic devices.

Materials Modelling and Design

Artificial sensors and actuators integrated with a passive elastic continuum provide a 'life-like' sensation and action/reaction capability for the elastic continuum. If the continuum is made of functionally graded materials (FGMs), the passive structural system transforms into an active functionally graded adaptive system. General theories for distributed sensors and actuators laminated on thin shell continua have been established. Distributed transducers for thin plates and plate laminates with piezoelectric layers are extensively found in literature. FGMs are a special kind of composite materials made up of two or more basic materials, whose material
properties vary according to a power law relation, and in recent years, FGMs have been extensively used in high temperature applications. These integrated FGM systems may also be deemed to represent piezoelectric skeletal materials, and this project aims to study these complex smart systems. Activities in this area are also closely intertwined with the program on MEMS modeling.

**Integrity, Reliability and Failure Modeling**

Electronic and engineering products are increasingly designed for service operation reliability by computational modeling techniques. Virtual modeling and simulation of product integrity, reliability and failure is a rapidly growing technology with major incentives in shortening the product design and development cycle time. Thermo-mechanical induced deformations, vibration fatigue, fracture integrity and interface delamination are some of the concerns in product reliability characterisation. The aim of this program is to develop integrated computational modeling and simulation techniques for characterising reliability and failure prediction in semiconductor devices, electronics packaging assembly, advanced materials system and integrity design in product systems.

**Meshless Methodology Development and Application**

Even though the finite element method (FEM) is arguably the principal numerical analysis tool of choice for the modelling and simulation of a wide-range engineering problems, it possesses certain disadvantageous features. These include repeated remeshing for tracking large dynamic deformation processes and the need for large storage and memory requirements due to the large number of nodal variables involved in FEM discretization. To overcome these problems, over the last few years, the meshless approach, often referred to as the next-generation numerical tool, has attracted much attention amongst researchers world-wide. Meshless methods do not possess the concept of a mesh and thus there is no requirement for mesh generation, which is replaced by a sprinkling of nodal points in the domain of interest. In general, meshless methods can be classified roughly into two groups, namely, those that require a background mesh such as Galerkin-based techniques and those that do not require a background mesh such as collocation techniques. In this program, both classes of techniques are explored. The main objectives here are twofold. Firstly, it is to develop new meshless techniques based on moving least squares and reproducing kernel approximates. Secondly, it is to apply these refined techniques to a wide range of problems, such as biomechanics, shell dynamics and smart materials modeling.

**Computational Nanoscience – Multiscale Simulation**

The current understanding of materials phenomena is based on a hierarchy of physical descriptions through space-time regimes of electrons, atoms (or molecules) and matter, which are described by theories based on quantum mechanics, statistical mechanics (molecular dynamics), and continuum mechanics. This naturally leads to a form of physical domain decomposition, namely: $A^3$ volumes where excitations due to electron activity must be calculated explicitly, e.g. using tight-binding (TB) methods; $nm^3$ volume scale regions where atomic activity can be approximated by empirical potentials, e.g. using molecular dynamics (MD) simulation; and $>\mu m^3$ volume scale regions where continuous displacement fields are suitable for good approximation, e.g. using finite element (FE) method. It is becoming more and more evident, especially with the advent of the nano-sciences, that it is impossible to fully understand material phenomena if the simulation is carried based on just one theoretical model alone. This project aims to develop and describe in detail the two handshaking regions so as to solve multiscale problems involving solid structures with internal and boundary singularities. Tribology issues such as interacting surfaces in relative motion will also be examined. Further, meshless point collocation techniques will be explored to replace the FEM for the macro domain.
Bio-Computing

Bio-informatics is an emerging scientific discipline that exploits information technology to answer biological questions. The research efforts in computational genomics focus on a genome wide protein structural study and drug design. State-of-the-art biomolecular modeling and drug design software's are applied to model three-dimensional protein structures from sequences and ligand-protein interactions. Protein modeling provides a valuable approach to complement the biological knowledge that can be obtained from experiments, and can also serve as a guide for experimental-planning for the systematic design of therapeutic agents for diseases. Efforts are also directed towards developing knowledge-based algorithms for identifying protein families and structurally conserved regions in sequence datasets.

We study systems biology by gathering genome data, compartmentalizing the genome data and creating algorithms using molecular sequence, structure, evolutionary tree and expression information to infer the functions of genes. Our work involves organizing genome data in an orderly manner based on simplest elements like introns and exons in relation to proteins, families, folds and class. We routinely use bioinformatics tools for sequence analysis, structure prediction and functional elucidation.

PUBLICATIONS

Selected list of publications:


CONTACT

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