Research Fellows and Research Projects (2003/2004)

HPCES programme

Dr Gao Xiangyang
Expertise: Molecular dynamics simulation, phase transformation, finite element method

Polynomial Optimization
Project Advisor (Singapore) : Assoc Prof Liu Guirong
Duration : August 2003 to August 2004

Project Abstract :
Biological membrane is an essential component of all living cells. Drug agents may have harmful side effect on the bio-membrane and affect its functions related on. Its interactions with bio-membrane received increasing interests in recent years. Lipid bilayer is usually treated as a simplified structure of bio-membrane. Due to the flexible nature of lipid molecules and the complex hydrophilic and hydrophobic interactions, computer simulation has emerged as a critical tool for modeling the lipid bilayer. This project adopts molecular dynamics simulation method to investigate structural properties of lipid bilayer that are temperature and pressure dependent, the interaction between lipid molecules and water, ion binding effects on the lipid bilayer, and the interactions between a few drug agents and lipid bilayers. A consistent force field has been setup for the targeted molecules.

Dr Han Deren
Expertise: Theory and applications of variational inequality problems

Polynomial Optimization
Project Advisor (Singapore) : Prof Sun Jie
Duration : November 2002 to November 2004

Project Abstract :
Optimization problems with polynomial have wide applications in industry and engineering and are very hard to solve due to nonconvexity of the objective function and/or the feasible set. Recently, some relaxation methods for this class of problems are proposed such as linear programming approximation and semi-definite programming approximation. We will study some new relaxation strategies for the problems.

Dr Kannan Balaji
Expertise: Combinatorial optimization, supply chain and electronic commerce

A Decision Support System for Strategic Inventory Placement in an Acyclic Supply Chain Network
Project Advisor (Singapore) : Assoc Prof Teo Chung Piaw
Duration : April 2003 to March 2004

Project Abstract :
Strategic inventory placement in a supply chain is a challenging and a well researched problem. In this research, we address the problem of developing a decision support system for strategically placing inventory in an acyclic supply chain network. When the guaranteed service times for the final stages (finished good stages) are input to the system, it recommends service lead times for each of the non-final stages (upstream stages of finished goods) that would minimize the inventory holding cost over the supply chain, based on the production lead time, the inventory holding cost, and, the demand, at each stage of the supply chain. The optimal inventory placement can be modeled as a mixed-integer programming problem. We also devise efficient algorithms to solve this problem.

Dr Liu Xin
Expertise: Computational mechanics, meshless methods

Research and Application of Meshless (Meshfree) Methods
Project Advisor (Singapore) : Assoc Prof Liu Guirong
Duration : May 2002 to May 2004

Project Abstract :
In recent year, research on meshless (meshfree) methods has made significant progress in science and engineering, especially in the area of computational mechanics. Meshfree methods based on radial basis function (RBF) have a clear advantage over other meshfree methods due to its simplicity and stability in field variable interpolation. However, traditional radial basis function methods result in fully-populated matrices, which limit its application in large scale practical engineering problems. This project aims to study meshfree methods using RBFs in a locally support domain, so that the system matrix becomes sparse and hence can be applied to more complicated problems. Two different formulation procedures based radial basis point interpolation method, namely Galerkin-based and collocation approaches, will be examined.

Dr Mi Dong
Expertise: Theoretical analysis of bio-systems

Protein Folding Mechanism
Project Advisor (Singapore) : Assoc Prof Liu Guirong
Duration : August 2003 to August 2005

Project Abstract :
Protein folding is one of the most complicated problems in structural biology. Although it is not yet possible to reliably predict the native structure of a protein from its sequence, the understanding of mechanisms governing protein folding, which also lead to better structure prediction algorithms, has progressed considerably. A number of mechanisms, such as “molten globule” model and “Folding Funnels”

model, etc, have been proposed to explain how naturally occurring proteins reach their native structures with a biologically relevant time scale. However, most of the mechanism only can qualitatively describe protein folding process. In this project, by using thermodynamics, kinetics and statistical methods, we will construct protein folding model which can give the quantitative information of protein folding.

Dr Rosales Fernandez Carlos
Expertise: Electromagnetic fields and devices, flow measurement

Dielectrophoretic Single Cell Trap Design Optimization

Project Advisor (Singapore)	:	Asst Prof Lim Kin Meng
Duration	:	September 2003 to September 2005

Project Abstract :
This project focuses on the development of the computational tools necessary to simulate the behavior of micron-sized particles in a dieletrophoretic trap. The objective is to gain a sufficient physical understanding to be able to predict with computer simulations which is the optimum design of the dieletrophoretic trap for a set of user specifications (temperature tolerance, flow rate, particular kind of particle that must be trapped). The problem includes the calculation of the electric forces, fluid flow forces and temperature fields on complex geometries, although my contribution will be mostly connected to the electric field, and more in particular, the development of a boundary element method for the accurate calculation of the electrical forces on the particle's surface.

Dr Wang Shengyin
Expertise: GA-based topology optimization, morphological representation global optimization methods, compliant mechanism

Topology and Shape Optimization of Structures by Evolutionary Algorithms

Project Advisor (Singapore)	:	Assoc Prof Tai Kang
Duration	:	March 2002 to March 2004

Project Abstract :
The ability to optimize the structural geometry of design artifacts is recognized as the next big step in design automation and will have a big impact in the CAD/CAE industry. Current design optimization software are mainly add-ons to existing CAE software, and as such do not represent a smooth integration between optimization and simulation. They also do not resolve the fundamental differences between the geometric data used in CAD and that used in CAE, and these differences are the main stumbling blocks that prevent design optimization from being applied routinely in engineering design and being developed into successful commercial software for industry. In this research, a fundamentally different approach towards the underlying geometry representation is being developed as an enabling technology to allow engineers to apply both optimization and simulation together in an intuitive and designer-friendly way. The capabilities and robustness of the techniques are to be established and demonstrated for engineering structures and components.

Dr Xing Xiuqing
Expertise: Aerodynamic design, flow field simulation and numerical optimization's application in turbomachinery

Optimization and Simulation of Aerodynamics Shapes using Simultaneous Perturbation Stochastic Approximation and CFD

Project Advisor (Singapore)	:	Assoc Prof Murali Damodaran
Duration	:	April 2001 to April 2003

Project Abstract :
The Simultaneous Perturbation Stochastic Approximation (SPSA) method has been demonstrated in literature for handling difficult multivariate optimization problems, and has recently attracted considerable attention in many different areas such as statistical parameter estimation, feedback control, simulation-based optimization, signal and image processing and so on. The primary strengths of this method are the ease of implementation, the lack of need for loss function gradient, theoretical and experimental support for relative efficiency. It is robust to noise in the loss measurements and has the ability to find a global minimum when multiple minima exist. The SPSA has being tested on several standard functions for comparative studies with other optimization methods. It is being assessed for constrained and unconstrained design of optimal aerodynamics shapes of the leading edges of turbo-machinery blades, airfoil sections, nozzle profiles. Objective functions optimized are evaluated using CFD solvers. Experiments are also done coupling it with other optimization methods to form hybrid methods. The effectiveness of this method over other optimization methods is also being assessed for multi-objective design optimization.

Dr Xuan Zhaocheng
Expertise: Numerical methods for partial differential equations

Output Bounds for Partial Differential Equations

Project Advisor (Singapore)	:	Assoc Prof Khoo Boo Cheong
Project Advisor (MIT)	:	Prof Jaime Peraire
Duration	:	December 2000 to December 2004

Project Abstract :
This project focuses on the development of methods for the efficient calculation of lower and upper bounds to outputs which are functionals of the solutions to partial differential equations. Such methods are extremely useful in engineering design where outputs, such as temperatures, displacements and stresses are needed at critical locations, provided of course that the methods are accurate, efficient and inexpensive. Obviously, coarse element discretizations are inexpensive but rather inaccurate, while fine element discretizations are accurate but expensive. The aim is to find methods which possess both accurate and inexpensive characteristics, and which can also be implemented with little difficulty in multiprocessor environments. In particular, the primary objective of this project is to extend the recent work of Patera and Peraire to fracture mechanics problems, where lower and upper bounds to stress intensity factors will be of importance to fracture-resistant design. This has been successfully achieved for stress intensity factors in homogeneous and bimaterial crack problems obtained with the displacement extrapolation method, and for J-integral with a novel method which can treat the quadratic functionals. Now we are computing the bounds to the exact values of J-integral.

Dr Yao Haiying
Expertise: Analysis of electromagnetic scattering, and radiation by using the fast algorithm

Modeling and Simulation for Metamaterials
Project Advisor (Singapore) : Assoc Prof Li Le-Wei
Duration : December 2002 to December 2004

Project Abstract :
A new artificial composite medium, called metamaterials has attracted more and more scholars. These materials have special characteristics those are not found in nature and not observed in the constituent materials. The properties of these composites are not determined by the fundamental physical properties of their constituents but by the shape and distribution of specific patterns included in them. There are various models for describing the characteristics of electromagnetic waves with metamaterials. In general, there are two kinds. One is to directly make use of the electromagnetic numerical simulation tools, such as method of integral equations (IEs) and finite different time domain (FDTD) method, to investigate the electromagnetic characters of the whole structure. The other is to evaluate the effective constitutive parameters of the composite structure, then develop numerical simulation tools to predict the electromagnetic performance of this complex medium. We present the second method and deduce the effective constitutive parameters by using quasi-static Lorentz theory and numerical simulation first. We will design the composites with special shaped inclusions those have special optical properties and a broad range of applications after we develop the simulation codes.

Dr Yao Zhenhua
Expertise: Molecular dynamics simulation of carbon nanotubes

Physical Properties of Carbon Nanotubes
Project Advisor (Singapore) : Assoc Prof Wang Jian-Sheng
Duration : October 2002 to October 2004

Project Abstract :
Carbon nanotube was discovered by S. Ijima in 1991, and was characterized by a lot of unique mechanical, electrical and optical properties. It has become a very active research field in recent years because of its potential applications in many areas. In this project molecular dynamics simulation method is adopted to study the mechanical, thermal properties and growth mechanism of carbon nanotubes and some new computation methods will be studied and parallelized algorithm will be developed as well. Parallelized molecular dynamics simulation software for carbon and silicon materials has been developed, and a fast and highly parallelizable neighbor list updating algorithm has been proposed and implemented in this software.

Dr Zhang Xiangkun
Expertise:
1. Numerical analysis on materials processing, such as casting solidification and heat treatment
2. Computational fluid dynamics
3. Level set method
4. Finite element method, meshfree method

Electrostatic Traps for Massively Parallel Single-Cell Manipulation
Project Advisor (Singapore) : Asst Prof Lim Kian Meng
Duration : September 2003 to September 2005

Project Abstract :
Microelectrode structures in AC electrokinetics can generate high electric field strength to manipulate, characterize and separate particles in suspending medium. It has been widely used in biological, pharmaceutical and medical fields. The goal of this project is to create arrays of thousands of addressable electrostatic traps to hold and arbitrarily sort single cell. The traps use dielectrophoresis (DEP) to create electrical barriers that trap cells, a phenomenon that has been used for over 30 years. The numerical method will be used to simulate the manipulation, characterization and separation of micrometer particles and provide the optimized for actual real-world use.

Dr Zhang Yongqiang
Expertise: Continuum mechanics simulation of carbon nanotubes

Mechanical Properties of Carbon Nanotubes
Project Advisor (Singapore) : Assoc Prof Liu Guirong

Duration : June 2003 to
June 2005

Project Abstract :
Since their first discovery and the establishment of new effective methods for production, carbon nanotubes (CNTs) have drawn a great deal of attention. As most potential applications of CNTs are heavily based on a thorough understanding of their mechanical behavior, the study of mechanical behavior of CNTs has been one topic of major concern. Besides the great deal of experimental works on CNTs, investigation of mechanical response of CNTs by theoretical modeling has been pursued. As experiments at the nanoscale are extremely difficult and atomistic modeling remains prohibitively expensive for large-sized atomic system, it is desirable to develop continuum theories that may overcome the limitations of atomistic simulations concerning both time and length scales. Thus, continuum mechanics models will continue to play an important role in the study of CNTs. In this project, some new continuum mechanics models will be developed to predict the mechanical properties of CNTs.