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FROM FUNDAMENTALS TO FUNCTION

the art of computational science

Powering Discoveries!

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from fundamentals to function

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Message from Executive Director:

It gives me much pleasure to present the IHPC Research Digest for FY2007.

It is an exciting time to be in computational science as modelling and simulation provide theorists with so many more opportunities to propel science and innovation in engineering. The advent of ever more powerful computers allows those in the field to simulate, and understand, with a high degree of fidelity, complex phenomenon and systems.

IHPC has over 130 technical staff from 20 different nationalities, 90% of whom hold Ph.D degrees in diverse disciplines such as physics, chemistry, computer science, materials science, mechanical-, chemical-, electronics- engineering and mathematics.

Our researchers have a common working language, which is to use an array of modelling and simulation techniques as well as computational tools to conduct research in a wide variety of scientific and technical problems in natural and engineered systems.

It is our aim to develop capabilities which traverse scales easily from ab initio to continuum, incorporating multiple physical phenomenon to better emulate complex natural and real systems.

The theme of this Research Digest is “From Fundamentals to Function – the Art of Computational Science”. As the name implies, it showcases our span of work in a spectrum of activities from basic science to applications.

We hope that this Research Digest will provide a better insight into our expertise, and how our research has advanced Science and Technology.

Dr Raj. Thampuran
Executive Director, IHPC

Introduction to IHPC

The Institute of High Performance Computing (IHPC) is a national research institute under the Agency for Science, Technology and Research (A*STAR). Established in 1998, IHPC is committed to enhancing Singapore's global competitiveness through innovative research in leading-edge computational science.

We are the host to the most powerful supercomputers in Singapore, which has grown proportionately in response to the burgeoning demand for resources from researchers over the past 7 years.

MISSION

IHPC's mission is to advance science and technology, and to develop leading edge applications, through high performance computing and computational science.

VISION

IHPC's vision is to provide leadership in high performance computing as a strategic resource for scientific inquiry.

ORGANISATION

There are four Research Programmes in IHPC. Each Research Programme is supported by a few teams that carry out research in focused areas:

ADVANCED COMPUTING PROGRAMME

- Advanced Software and Architecture
- Adaptive and Collaborative Computing
- Digital Modelling and Visualisation

COMPUTATIONAL MATERIALS SCIENCE AND ENGINEERING PROGRAMME

- Computational Chemistry
- Multiscale Modelling
- Solid State Electronics and Nanostructures

ENGINEERING SOFTWARE AND APPLICATIONS PROGRAMME

- Engineering Software
- Electronic Systems

LARGE-SCALE COMPLEX SYSTEMS PROGRAMME

- Engineering Mechanics
- Computational Fluid Dynamics
- Heterogeneous Coupled Systems
- Biophysics

FUNDAMENTALS

FUNDAMENTALS

Some 50 years ago, a physicist named J.C. Slater challenged scientists to calculate and predict materials function and properties from first principles instead of observation through conventional experimentation. However his vision is largely unrealised to this day. For instance, materials design is still a predominantly trial-and-error exercise.

The traditional experimental approach is no longer an efficient way to produce new materials and devices in today's world - new research strategies are needed to accelerate discovery and innovation.

THERE ARE TWO PARTS IN THIS SECTION:

NEW METHODS - showcases new methodologies we have developed to understand the physical and chemical properties of materials.

NEW MATERIALS - showcases our unique capabilities in discovery of new materials.

NEW METHODS

- Nucleation and Crystallisation
- The Physics of Colour – Probing Light-Induced Excited States in Nanoparticles
- Complex Systems
- Multiscale Modelling
- Plasmonics
- Smoothed Particle Electromagnetics and Its Application in Computational Nanometre-Scale Optics
- Materials Observed through a Virtual Microscope: Molecular Dynamics Simulation

NEW MATERIALS

- Interfacial Chemistry
- Functional Materials
- Nanosystems
- Carbon Nanotubes and Its Applications

Representative Publications

Chee C.Y. "Noise induced spontaneous solidification in pure material" 15th International Conference on Crystal Growth (2007)

Chee C.Y., Lee L., Rosales C. and Whyte D. "Observation of a Nonlinear Crystallization Process from Phase Field Modeling" 9th US National Congress on Computational Mechanics (2007)

FUNDAMENTALS – NEW METHODS

NUCLEATION AND CRYSTALLISATION

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THE PROJECT

Natural events such as formation of ice, a gemstone or bubbles in a soda are driven by the physics of nucleation and crystallisation. The nucleation and crystallisation process is relevant in varied fields such as materials science, microbiology, meteorology and even cosmology. Our research is focused on the process of nucleation and crystallisation relevant to material science.

The nucleation and crystallisation process is of industrial importance because many modern applications depend on materials with highly tailored properties. Depending on the application, different end products of crystallisation such as defect free crystals, fine amorphous powders, small clusters with controlled size distribution, glass phases, meta-stable structures, novel microstructures and fine particles in a suspension are sought by the industry. Hence, obtaining those optimum properties especially on an industrial scale, requires a deep understanding of the physics of nucleation and the influence of various processing variables.

Crystal formation and growth is an outcome of the interplay between different aspects of physics such as atomic interactions, fluid mechanics, thermodynamics, and phase transformation. The study of such a heterogeneous system involves understanding the underlying physical processes at various length and timescales. Our research goal is to gain understanding of this problem by simulating the microscopic events using atomistic modelling such as molecular dynamics and Monte Carlo methods; the mesoscopic physics by continuum models; and the macroscopic process of large crystal interactions using statistical methods such as population dynamics. Finally, empirical control equations that evolve from the outcome of these studies will be sought. As our nucleation and crystallisation theories develop, specific systems will be investigated in validation studies.

Atomistic simulations provide insight into different measures such as nucleation rates, incubation time and interfacial mobility. These measures are used in coarse grained continuum simulations as input parameters, to gain a better understanding of the details such as interfacial structure, shape of the crystal and macroscopic coarsening rates. Statistical methods, in turn, use this information to study an ensemble of large number of clusters/crystallites, the evolution of a distribution of crystal sizes and the influence of control parameters like temperature and pressure at large scales.

These methods are also used to study the interaction of the crystals with the medium and its degradation due to collision, attrition or fragmentation. The modelling of the nucleation and crystallisation process at these varied length and time scales would lead to an empirical model as a function of the process parameters, with predictive capabilities on a large scale. In this project, we restrict our attention to crystallisation processes from solution, which is relevant to the chemical and pharmaceutical industries.

The modelling of the microscopic processes during nucleation involves knowledge of the inter-atomic interactions which are obtained from calculations using *ab initio* methods. We will look to our colleagues in the Computational Chemistry Team to assist us in developing these potentials. Our collaboration with colleagues in the Advanced Computing Programme helps in the code development, optimisation and visualisation. Our interaction with researchers in other A*STAR research organisations and universities helps us in gaining new insights on various aspects of the project and crystallise the research goal and direction.

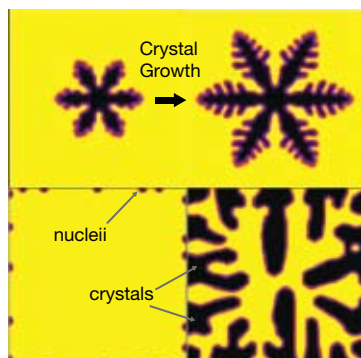


Fig.1 Crystal Growth

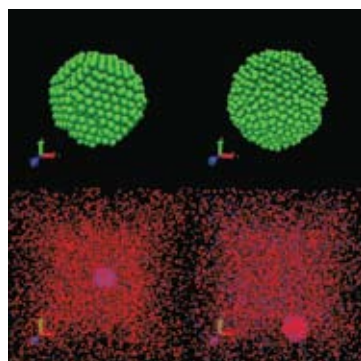


Fig.2 Cluster Dynamics

THE PHYSICS OF COLOUR - PROBING LIGHT-INDUCED EXCITED STATES IN NANOPARTICLES

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THE PROJECT

Light and nanoparticles are at the core of critical technologies in fields ranging from energy and environment to medicine. These technologies, such as hydrogen production through water splitting, solar cells, photocatalytic decomposition of pollutants, cancer detection and therapy, or integrated silicon optoelectronic systems, share a common denominator, namely they depend on the fate of light-induced excited states.

Upon absorption of light, a system is brought into an excited state by forming a neutral pair electron-hole. The electron, initially contributing to the bonding between atoms, is transferred to a higher energy level, leaving behind a positively charged hole. The absorption, which gives also a material its colour, is a fast process (in the order of 10^{-15} s). The relaxation to the ground state, however, is slower and can take different pathways. The most dramatic one is the breaking apart of the system.

One familiar example is the decomposition of oxygen and ozone under the action of UV light in the higher atmosphere, thus preventing harmful radiation to reach the surface of the earth. This applies to particles too, as observed in the photodecomposition of silver halide particles into silver metal, which is at the origin of the photographic process. In fact, most nanosystems undergo some kind of structural modification under the action of light, from simple bond stretching to bond breaking and surface reconstruction. The effect appreciably influences the optical properties of nanoparticles, and can sometimes even dominate the quantum confinement effect, as in the case of the luminescence in silicon nanoparticles. Other critical properties such as the electron-hole separation and charge transfer are also affected by the response of the system to light.

Our research focuses on the use of computational methods to simulate the origin of optical properties of nanoparticles.

While methods based on the density functional theory (DFT) are popular, they are more appropriate to describe the ground state. The many-body perturbation theory (GW approximation) is the method of choice to calculate the excited states; however the technique is computationally expensive.

The Quantum Monte Carlo (QMC) techniques, while less accurate, provide a better scaling with the number of electrons in the system, and clusters with a diameter up to 2 nm can even be described. The QMC method samples the many-electron wavefunction using a stochastic approach and the electron correlation effects are included precisely in the calculation of the total energy. On the other hand, the geometry of the system, in its ground state or excited states, can be optimized using the DFT method. The combination of DFT and QMC is a powerful tool to explore the light-induced excited states in nanoparticles.

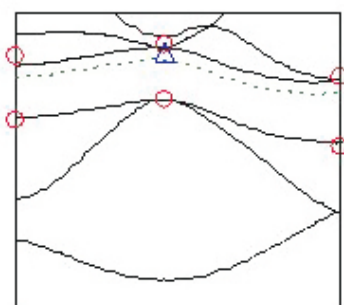


Fig.1 Band structure of bulk silicon. Excitation energies calculated using the GW approximation (triangle), the QMC method (circle) and the DFT method (dashed line).

Representative Publications

Rosales C., Whyte D.S. and Cheng M. "A Massively Parallel Lattice Boltzmann Method for Large Density Ratios" 7th Asian CFD Conference Bangalore, India (2007)

FUNDAMENTALS – NEW METHODS

COMPLEX SYSTEMS

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THE PROJECT

Imagine a magic box that supports a perfect vacuum. Now consider a well characterised droplet of Newtonian (simple) fluid in the middle of the box. If we apply an external force to the droplet, it is possible to accurately predict the motion of the droplet. Knowledge of Newtonian mechanics is sufficient as the droplets behave like non-deformable, solid particles. Suppose additional droplets are now distributed randomly throughout the box. As long the droplets do not collide, their motion under an external force can be still accurately predicted.

We can extend the problem by replacing the vacuum with a different Newtonian fluid. The droplets are now suspended in a medium – we have an emulsion. While the mechanics of an individual droplet are well understood we cannot make an immediate prediction as to how the swarm of droplets will behave.

There are some *knowns* – the hydrodynamic forces in each fluid; the transfer of momentum between the different fluids; and the forces that arise at the interface of the fluids. However, there is now an underlying connectivity between all the droplets. Depending on the concentration of droplets in the suspended fluid we can see non-linear effects. That is, small changes in microstructure of a fluid can lead to significant changes in the bulk fluid.

For example, in our emulsion, for low concentrations, the bulk fluid has a viscosity that is constant and close to that of the suspending medium when a variable force is applied to the fluid. At some critical concentration the viscosity becomes shear thinning – the fluid flows with less resistance to an applied force.

Everyday products which exhibit complex behaviour include mayonnaise, ice cream, chocolate, toothpaste, ketchup and shampoo. Decades of research have been put into trying to better understand these fluids so as to optimise production systems.

Experimental studies, sophisticated mathematical models and numerical tools have been brought to bear on the problem. Taking a computational approach we will investigate the physics of complex fluids. Our goal is to understand how the interplay of disperse fluids and the connectivity of the fluid can give rise to complex behaviour.

Through the years various computational techniques have been developed to investigate the flow of multiphase fluids, most are based on finite-volume or boundary-element methods. Continual improvements of these techniques enable very accurate predictions of how an individual droplet/bubble will react to a specified flow field.

Computational limitations still hold back standard techniques. Thus, there has been little advancement in methodologies to study how systems of many droplets/bubbles interact – researchers have focused on extending accurate, single droplet/bubbles deformation simulations to bulk fluid models. In the last few years the Lattice Boltzmann method (LBM) has matured as a tool for the study of multiphase systems. We will exploit the inherent computational efficiency of LBM to simulate systems that include many dispersed droplets/bubbles.

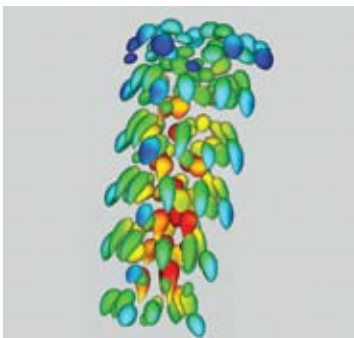


Fig.1 Bubble Column

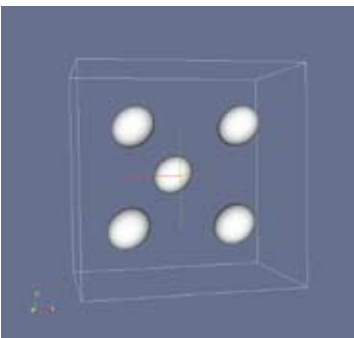


Fig.2 Sheared Emulsion

Representative Publications

Gan C.K., Feng Y.P. and Srolovitz D.J. "First-principles calculation of the thermodynamics of In_xGa_{1-x}N alloys: Effect of lattice vibrations" *Physics of Plasmas* **13(6)** 063102 (2006)

Gan C.K. and Srolovitz D.J. "First-principles study of wurtzite InN (0001) and (0001)over-bar surfaces" *Physical Review B* **74(11)** 115319 (2006)

FUNDAMENTALS – NEW METHODS

MULTISCALE MODELLING

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THE PROJECT

Modelling of real materials is a challenging enterprise since it involves multiple time and length scales. The multiple time scale demands that one has to run a simulation long enough to capture the correct time-averaged properties over different time scales. The length scale poses another challenge in that the system size that is used must be large enough to capture all spatial irregularities within the materials. Modern first-principles methods have had tremendous successes to treat relatively small-size (< 200 atoms) systems. This is because very high accuracy could be derived from first-principles calculations.

To simulate larger systems (> 1000 atoms), one obviously has to find other alternatives. In order to bridge different time and length scales, it is necessary to combine different computational techniques to enable multiscale modelling so that a difficult problem can be solved. There are in general two categories in multiscale modelling; the first is to start from the smallest scale and move toward a larger microscopic scale, while the second approach is to start from a larger scale (usually continuum or mesoscale) to the microscopic level.

The computational strategy that we have adopted is based on the former approach, i.e., we start from the smallest scale and move toward a larger scale. There are different multi-scale approaches that are being adopted by the Multiscale Modelling Team. These are (i) hybrid of the tight-binding method with the force-field method, and (ii) phase-field modelling.

We have already embarked on the research to combine the tight-binding approach with force-field methods. The tight-binding parameters are obtained by fitting the results obtained using first-principles density functional theory. We are currently performing large scale atomic dislocation dynamics to validate the dislocation model as well as the tight-binding approach. Once this task is accomplished, one then can establish a multiscale approach where the tight-binding approach will be coupled with force-field methods.

In this multi-scale approach, the region that requires very high numerical accuracy will be treated by the tight-binding method and the region that are less critical (e.g., near perfect lattice structure) will be treated by force-field methods. One of the challenges is the implementation of an efficient hand-shake algorithm to address regions treated by both the tight-binding and force-field methods.

The phase-field modelling is yet another effort carried out by the members of the Multiscale Modelling Team. In this approach, the free energy functionals are estimated based on physical grounds. A free energy functional may involve different parameters that could be determined from experimental data or accurate first-principles or tight-binding calculations. By minimizing the free energy functional as functions of physical variables such as temperature, one could extract useful physical properties such as transition temperatures. One may also study the time-evolution of the microstructures based on phase-field modelling.

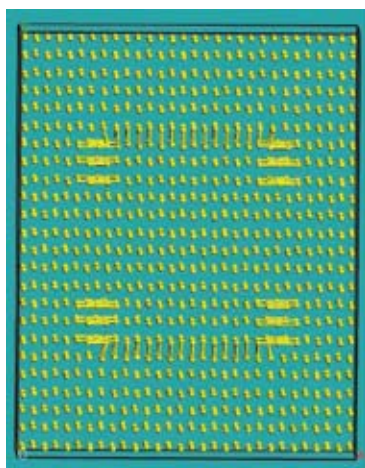


Fig.1 A dislocation model of 1488 Al atoms. The lower and upper portions are mirror images of one another so that full periodicity can be restored for the super-cell calculation. Each portion depicts two partial dislocations at both ends (bonds are used to join atoms that are close to one another) separated by a stacking fault region. The four partial dislocation lines are normal to the page

Representative Publications

Chu H.S., Ewe W.B., Li E.P. and Vahldieck R. "Analysis of sub-wave length light propagation through long doublechain nanowires with funnel feeding" *Optics Express* **15(7) 4216-4223** (2007)

FUNDAMENTALS – NEW METHODS

PLASMONICS

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THE PROJECT

A plasmon is the quasiparticle resulting from the quantisation of plasma oscillations just as photons and phonons are quantisations of light and sound waves, respectively. Thus, plasmons are collective oscillations of the free electron gas density, often at optical frequencies. Plasmons that are confined to surfaces and which interact strongly with light are known as surface plasmons. The study of this phenomenon is known as plasmonics. Plasmonics can be considered to be a truly nanophotonic module for communications, imaging and spectroscopy by exploiting localised and propagating surface plasmons that access nanometer-scale wavelengths at optical frequencies.

Plasmonics has a variety of potential applications. Plasmonic nanowires can be much thinner than conventional wires, and could support much higher frequencies. Thus plasmonics has been considered a means of transmitting information on computer chips. The plasmonic resonance of metallic films, several interacting metallic nanorods, nanowires or nanoholes can be used to guide, filter, switch or manipulate light. The availability of extremely small wavelengths in plasmonics means that it could be utilised in high resolution lithography and microscopy. In addition, the surface-plasmon-based sensors also find uses in gas sensing, biological environments such as immuno-sensing and electrochemical studies.

We focus on the modelling and analysis of plasmonic nanostructures for various applications such as near field optics, guiding light, and nanosensor. Several in-house codes based on frequency- and time-domain methods such as the surface and volume integral equations, scattering matrix method as well as finite-difference time domain method have been developed at IHPC. These methods enable full characterisation of the optical properties of plasmonic nanostructures. Using in-house codes such as the surface integral equations, some of the plasmonic applications which we have investigated are shown in the figures.

The result, in Figure 1, shows that the strong field enhancement, like-dipole, can be obtained at the surrounding area of an elliptical silver nanowire having the overall size of 40 nm x 10 nm. The plasmonic waveguide consisting of coupled silver nanowires, as shown in Figure 2, is useful for guiding light at the tiny cross section of 50 nm. The last result, in Figure 3, demonstrates that the silver nanowire with the radius of 25 nm can be used as nanosensor to detect its surrounding nano-environment. The shift of extinction peak is due to the variation of the reflective index of surrounding mediums.

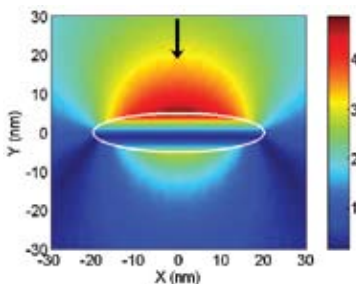


Fig.1 Near field intensity is strongly enhanced around the elliptical silver nanowire at resonance

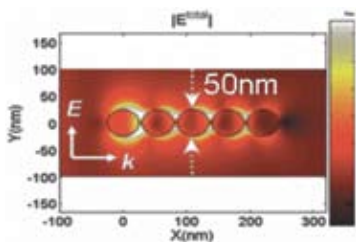


Fig.2 Nanoscale plasmonic waveguide for guiding light at the cross section of 50 nm

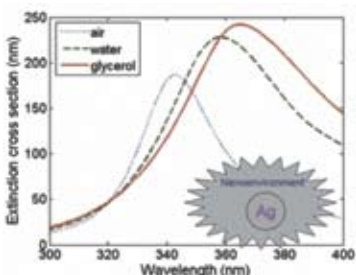


Fig.3 Plasmonic nanowire for nanosensing application.

SMOOTHED PARTICLE ELECTROMAGNETICS AND ITS APPLICATION IN COMPUTATIONAL NANOMETRE-SCALE OPTICS

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THE PROJECT

At present, substantial research effort is directed towards bridging the dimension mismatch between optical and the much smaller electronic components, thus allowing broad-band on-chip interconnection that is less affected by thermal and power consumption problems. This requires the development of optical devices of several nanometres in size. One emerging technology that is anticipated to allow the confinement of light to such dimensions is Plasmonics. Electromagnetic waves can propagate along the surface of conducting materials as a result of the interaction with the free electron gas. Since this allows sub-wavelength confinement of light, plasmonics will be a promising technology that enables a significant step in the size reduction of opto-electrical integrated circuits, which would result in the development of smaller, faster and more power-efficient electronic devices in the future.

The development of this technology and potential components will require efficient and reliable simulation tools. The simulation approaches that are currently in use for such structures assume material properties that are equal to those of bulk materials and do not account for the variation of these properties at very small physical dimensions. Here, the movement of charged particles plays an increasingly important role. Whether traditional – macroscopic – material models still hold at dimensions of several nanometres, where features are composed of no more than a few atoms, yet needs to be answered to the full.

Smoothed particle electromagnetics (SPEM) – an extension of the established smoothed particle hydrodynamics (SPH) method – is anticipated to incorporate moving particles in the simulation of electromagnetic fields. Being a mesh-free method, SPEM does not require a predefined topological relation between the points in which the electric and magnetic fields are computed. This feature makes it attractive for applications, where the geometrical or electrical properties vary over time.

Our current research focuses on improving the accuracy and reliability of this method in dynamic implementations and assessing its applicability to various types of electromagnetic problems at a nanometre scale. For this purpose, time- and frequency-domain formulations are developed and applied to conventional electromagnetic simulations. This requires the implementation and testing of consistency restoring approaches that aim at eliminating the inherent accuracy deficiencies of this method. After the introduction of moving charges, its results can be compared to those obtained by conventional methods, which is anticipated to allow a judgement of their validity at microscopic dimensions.

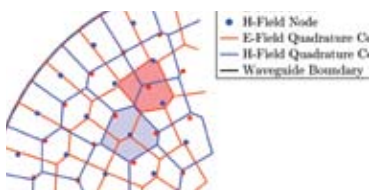


Fig.1 Partitioning of a hollow circular waveguide cross-section with the help of a Voronoi diagram for the numerical integration of the electric and magnetic fields. The conformal perfect electric conductor boundary is represented by means of fictitious nodes outside the computational domain that are assigned field values such that the interpolated fields fulfil the respective boundary conditions.

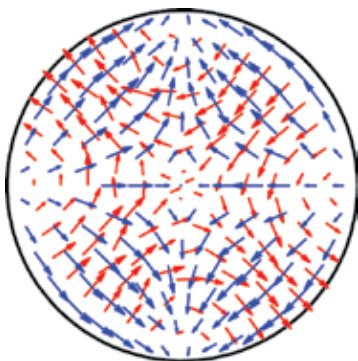


Fig.2 TM_{12} mode in a hollow circular waveguide computed as an eigenvector of the smoothed particle electromagnetics system matrix.

References

- 1 Marco Klähn, Abirami Seduraman, Ping Wu
- 2 Michael B. Sullivan, Jianwei Zheng, Ping Wu

FUNDAMENTALS – NEW METHODS

MATERIALS OBSERVED THROUGH A VIRTUAL MICROSCOPE: MOLECULAR DYNAMICS SIMULATION

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THE PROJECT

Computer simulations help us to uncover the underlying mechanisms that determine macroscopic features of various materials. Equipped with these insights, we are striving to predict new useful materials. One important tool for the simulation of materials is molecular dynamics, which allows us to observe the very details of a material.

Most of molecular dynamic simulations are done on an atomic level of detail. The dynamics of the atoms are evaluated at a chosen temperature and pressure, using Newton's equation of motion. This evaluation is governed by the potential energy of an empirical classical model for the simulated material. In this model, all atomic nuclei in the material are explicitly represented as point-like mass-particles, while electrons are described implicitly by springs that connect the nuclei

Using this approach, it becomes possible to simulate materials consisting of hundreds of thousands of atoms on a time scale of several nanoseconds and to derive from the simulation, many properties of the material.

We apply molecular dynamics to simulate a variety of different materials. In one project we study the properties of ionic liquids¹. An ionic liquid is a molten salt with a low melting point, which in some cases is below room temperature. While more eco-friendly, these fascinating new liquids can be used e.g. as catalysts, as separators for liquid compound mixtures and as filters for gases, just to mention a few applications.

We simulate ionic liquids with guanidinium-based cations (Figure 1) to learn how their properties are constituted by their atomic structure and energetics. Based on the simulations (Figure 2), we were able to develop a model for self-diffusion in ionic liquids, a dynamic property that is also tightly related to viscosity and conductivity. Analyzing the heating and vaporisation of ionic liquids, we were also able to understand how energetics influences the dynamics of the liquids and how both are related to atomic structures. In the next step, these insights will help to tailor new ionic liquids with desired properties.

Another project is devoted to the polarisation of ferroelectric polymers². Ferroelectric materials polarize due to an internal aligning of molecular dipole moments. Such materials are suitable for many applications such as memory units in computer RAM, medical ultrasound devices and fire sensors for instance.

The use of ferroelectric polymers in particular is promising due to their inertness, flexibility, low density and ease of fabrication. We simulate crystals of the ferroelectric polymer PVDF and study how temperature affects the polarisation of the crystal. We found the minimum temperature (critical temperature) that is required to disrupt the internal self alignment of dipole moments that leads to a complete loss of polarisation. We use this temperature as an essential parameter for a macroscopic model to analyze the response of the polymers to an external electric field.

The two introduced projects demonstrate that a look through this virtual microscope with molecular dynamics simulations onto the atomistic details of materials help us to understand the origin of their macroscopic properties. This knowledge is essential for the design of new materials.

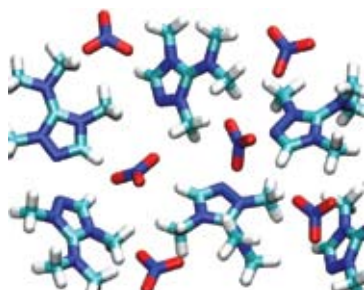


Fig.1 One of the simulated ionic liquids consisting of cyclic guanidinium-based cations and nitrate anions

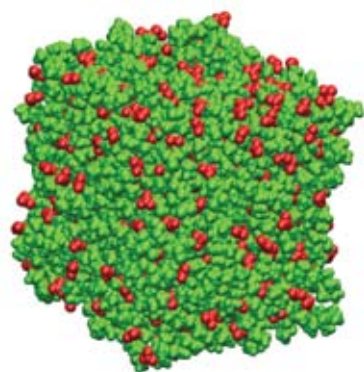


Fig.2 Simulation of 500 ion pairs in an ionic liquid with bulky cations in green and compact anions in red.

Representative Publications

Dai, L. and Tan V. B. C., et al. "Large scale ab initio molecular dynamics simulations of hydrogen-induced degradation of Ta diffusion barriers in ultralow-k dielectric systems." *Applied Physics Letters* **90(3)** 032906 (2007)

Yong K.S. and Zhang Y. P., et al. "Chemisorption of pentacene on Si(111)-7 x 7 studied via scanning tunneling microscopy and density functional theory." *Journal of Physical Chemistry C* **111(11)** 4285-4293 (2007)

Zhang, J. and Loh K.P., et al. "Adsorption of molecular oxygen on the walls of pristine and carbon-doped (5,5) boron nitride nanotubes: Spin-polarized density functional study." *Physical Review B* **75(24)**, 245301(2007)

FUNDAMENTALS – NEW MATERIALS

INTERFACIAL CHEMISTRY

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THE PROJECT

The Computational Chemistry Team at IHPC is studying the behaviour of materials at various kinds of interfaces. These materials are especially important in the electronics industry where many types of materials are squeezed together.

One application involves dielectric systems comprising Cu and ultralow-k (ULK) polymer dielectrics ($k < 2.4$) that are used in 65 nm interconnects. Currently, Ta is added on top of a surface of SiC to prevent copper from migrating into the SiC. In this work, we used Carr-Parrinello molecular dynamics (CPMD) to study how this barrier layer of Ta works. When hydrogen impurities were introduced into the system, the barrier layer broke down from an ordered and crystalline system to a loose amorphous system. This breakdown became ineffective in preventing the copper from migrating into the SiC.

In another study, we looked at an organic-inorganic interface that combined the traditional silicon substrate with new organic molecules that possessed unique electrical or optical properties. These organic molecules were typically pi conjugated and the one that we studied was pentacene, which is made up of 5 fused benzene rings.

By using density functional theory (DFT), we were able to identify the most favourable orientation on the silicon (111) 7x7 surface. We found that there was covalent bonding between the carbon-based pentacene and the silicon surface. This was somewhat surprising as it resulted in a loss of aromaticity. The calculations have led to a better understanding of the relative energetics of various orientations between the pentacene and the surface.

Lastly, we explored the adhesion of oxygen molecules on pure boron nitride nanotubes as well as carbon-doped boron nitride nanotubes to find the strength of the adhesion as well as the effect on the electronic properties of the nanotube. We found that oxygen did not form stable structures on the pure system but it did on the carbon-doped system. We also observed changes in the band structure with the introduction of the oxygen molecule on a particular carbon-doped location impart metallicity on the nanotube.

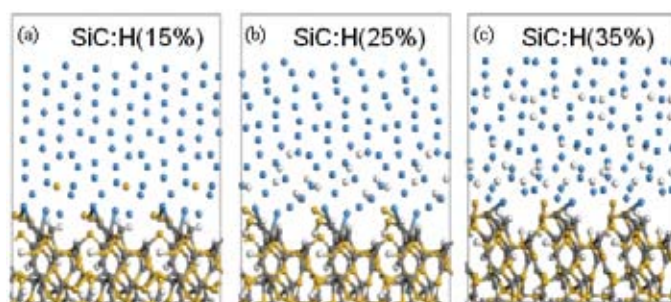


Fig.1 Structures of Ta atoms above three $\text{Si}_x\text{C}_y\text{H}_z$ amorphous surfaces of H molar percentages of (a) 15%, (b) 25%, and (c) 35%. Depositions were carried out in two successive batches of 16 Ta atoms each via a 200 ps CPMD simulation at 500 K.

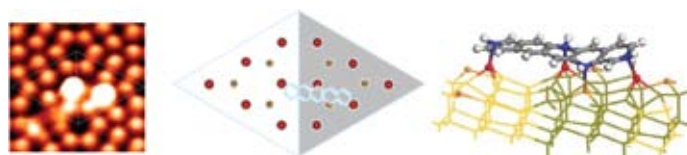


Fig.2 Experimental STM of pentacene on Silicon surface is shown in the left panel. The centre panel shows the attachment position that can be compared to experiment and the right panel shows details of the fully optimized structure.

Representative Publications

Ong K. P., Wu P., Liu L. and Jiang S.P. "Optimization of electrical conductivity of LaCrO₃ through doping: A combined study of molecular modeling and experiment" *Appl. Phys. Lett.* **90**, 044109 (2007).

Jiang S.P., Liu L., Ong K.P., Wu P., Li J. and Pu J. "Electrical conductivity and performance of doped LaCrO₃ perovskite oxides for solid oxide fuel cells" *Journal of Power Sources* in press. (2007).

Zhang J., Wu P., Ong K.P., Lu L. and Shu C. "Electronic properties of A-site substituted lead zirconate titanate: Density functional calculations" *Phys. Rev. B* **76**, 125102 (2007).

Ong K.P., Bai K.W., Blaha P. and Wu P. "Electronic structure and optical properties of AFeO₂ (A = Ag, Cu) within GGA calculations" *Chem. Mater.* **19**, 634 (2007).

FUNDAMENTALS – NEW MATERIALS

FUNCTIONAL MATERIALS

INVESTIGATORS

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THE PROJECT

We are studying different functional materials that can be used for the fabrication of fuel cells. Solid Oxide Fuel Cells (SOFC) are electrochemical devices which directly convert chemical energy to electricity with very high efficiency (see Figure 1). However, the performance and stability of a SOFC are critically dependent on the activity and structural stability of various cell components such as the electrolyte, anode, cathode and interconnects. Lanthanum chromite-based perovskite oxides have been investigated as interconnects for high-temperature SOFCs and power stations due to the high stability against oxidizing and reducing environment and good electrical conductivity. In order to enhance the performance of LaCrO₃ for such high temperature applications, optimisation of the electrical conductivity of LaCrO₃ is required.

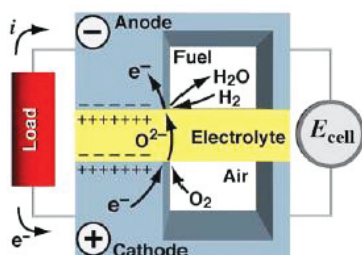
Substitution on the A and B sites with alkali earth and transition metal elements modifies the electronic structure of the oxides and shows interesting catalytic properties. For example, doping a small amount of divalent cation Sr²⁺ (about 0.1%) in place of La³⁺ will significantly reduce the optical gap of LaCrO₃, suggesting an increase of electrical conductivity as well. The main objective of our work is to optimize the electrical conductivity and to understand the mechanism of improvement in electrical conductivity of LaCrO₃ by screening all Group IIa elements, M²⁺ (Be, Mg, Ca, Sr, Ba, Ra) as a substitution dopant to the La site in LaCrO₃ (see Figure 2). We have applied molecular modelling to shorten the candidate list so that more focused experiments may be carried out efficiently.

Another area that we are interested in is multiferroics. They are materials that are both ferroelectric and magnetic. They are rare because in most ferroelectrics such as BaTiO₃, the ferroelectricity is driven by a hybridisation of empty *d* orbitals with occupied *p* orbitals of the octahedrally coordinated oxygen ions. The mechanism requires empty *d* orbitals and thus cannot lead to multiferroic behaviour. This is the so-called "d₀ ness" criterion.

However, "d₀ ness" does not rule out other possible ways of achieving multiferroics in the magnetic perovskite oxides and related materials. For examples, the multiferroic property of the widely studied BiFeO₃ is achieved by making use of the stereochemical activity of the lone pair on the large (A-site) cation to provide the ferroelectricity, while keeping the small (B-site) cation magnetic.

A second route to multiferroism is provided by 'geometrically driven' ferroelectricity, which is compatible with the coexistence of magnetism; the anti-ferromagnetic ferroelectrics YMnO₃ and BaNiF₄ fall into this class. The recent success of ferromagnetism in diluted magnetic semiconductors (DMS) or dilute magnetic oxide (DMO), also provides a another potential way for multiferroics by introducing dilute concentrations of magnetic species to ferroelectric oxide, thereby harnessing the benefits of a magnetic response without significantly affecting the ferroelectricity of the non-magnetic host.

The quest for multiferroic material by doping magnetic species in ferroelectric material, for example BaTiO₃ crystals, requires first a thorough understanding of the nature (charge state, local symmetry, and electronic structure) of the defects/impurities present in these materials, and of ferromagnetic and ferroelectric coupling as well as their interaction with light. To this end, IHPC has initiated a series of first principles calculations in cooperation with NTU as the experimental partner. Most of work focused on the role of oxygen vacancy in mediating orbital and spin order.



Cathode charge transfer:
 $O_2(g) + 4e^-(c) \rightleftharpoons 2O^{2-}(e)$

Anode charge transfer:
 $H_2(g) + O^{2-}(e) \rightleftharpoons H_2O(g) + 2e^-(a)$

Net:
 $H_2(g) + \frac{1}{2}O_2(g) \rightleftharpoons H_2O(g)$

Fig.1 Structure of one Solid Oxide Fuel Cell

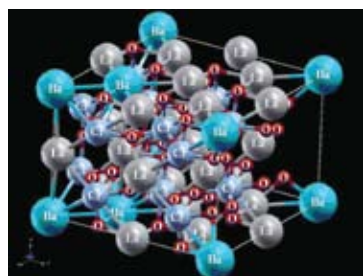


Fig.2 Crystal structure of $La_{1-x}MxCrO_{3-x/2}$ (M=Ca, Sr, Ba)

Representative Publications

Koh S.J.A. and Lee H.P. "Shock-induced localised amorphization in metallic nanorods with strain rate dependent characteristics", *Nano Letters* **6** (10) 2260-2267 (Oct 2006)

Koh S.J.A. and Lee H.P. "Molecular dynamics simulation of size and strain rate dependent mechanical response of FCC metallic nanowires" *Nanotechnology* **17** (14) 3451-3467 (Jul 2006)

FUNDAMENTALS – NEW MATERIALS

NANOSYSTEMS

INVESTIGATOR

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THE PROJECT

Nanowire systems represent the smallest possible dimension for electrical, chemical, thermal, optical, magnetic and mechanical wave transport. The transitional group of face-centred cubic (FCC) metals displays a rare combination of high ductility and mechanical strength, with good resistance to corrosion. Hence, they are often employed in harsh physical, chemical and biological environments. Current research is largely focused on the study of their electrical, chemical, thermal, optical and magnetic properties, neglecting a crucial vein – the study of their mechanical properties. As metallic nanowire systems are frequently placed in harsh ambient environments, studies on its mechanical response is mandatory.

We at Nanosystems@IHPC have conducted a series of computational studies on the mechanical static and dynamic responses of single-crystalline platinum (Pt), and gold (Au) nanowires and nanorods. We have adopted molecular dynamics (MD) simulations, using the many-body Sutton-Chen potential, for these studies. Our simulations showed that, due to the absence of defects, single-crystalline metallic nanowires could achieve tensile strength in the giga-pascal region (10^9 N/m²) under static loading. They undergo quasi-periodic stress-strain cycles, display superplastic behavior after first yield, and rupturing at more than 50% strain. The Young's modulus and Poisson ratio of the nanowires were not significantly different from the bulk properties.

An interesting phenomenon known as "strain-induced melting" was observed for the nanowires. It was observed that, at sufficiently high strain rates, the nanowires underwent phase transformation. The crystalline-ordered FCC structure was phase-transformed into a disordered amorphous structure, that is, a nano-metallic glass structure was formed in the absence of the thermal annealing process. This curious phenomenon is unique only at nanoscale as, at this size scale, the fusion of enthalpy (i.e. the amount of energy required to hold the atoms together) is greatly reduced.

This reduced enthalpy of fusion allowed the energy supplied by a sufficiently high strain rate (> 100 m s⁻¹), to physically break the metallic bonds and send the originally ordered structure into disarray. This would not have been possible for bulk materials with a very much higher enthalpy of fusion. Nanowires could therefore be "mechanically-melted" at room temperature. It was also discovered that the melting is localised, and the location of the melted region could be easily controlled by varying the strain rate. The amorphous structure could then be stretched to two times more its original length ($>100\%$ strain), displaying both exceptional strength and superplasticity. "Strain-induced melting" is a good way to produce nano-metallic glasses, due to advantages such as localisation and controllability.

We have further discovered that the strain wave propagation speed is size-dependent, which was observed to be much faster than that predicted from the continuum 1D wave propagation equation. This was attributed to the significant proportion of surface atoms in nanowires with characteristic sizes smaller than 4.0 nm, resulting in the presence of inherent surface stresses. The enhancement in wave propagation speed was found to follow a second-order relationship with the surface stresses. We have planned for future studies investigating on other modes of nanowire deformation like bending and twisting, and the mechanical response of other nanowire systems like nanorings, nanosprings, nanochains and nanoropes.

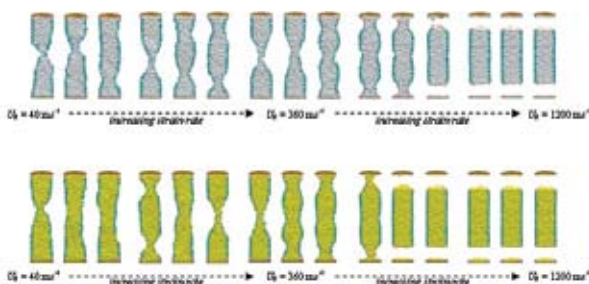


Fig.1 The evolution of neck locations of platinum (top) and gold (bottom) nanowires as the strain rate was varied from quasi-static to dynamic shock. The location of the amorphous neck can be controlled by the rate of strain.

Representative Publications

Reddy C.D., Lu C., Rajendran S. and Liew K.M." Free vibration analysis of fluid-conveying single-walled carbon nanotubes", *Applied Physics Letters*, **90**, 133122 -1 (2007)

FUNDAMENTALS – NEW MATERIALS

CARBON NANOTUBES AND ITS APPLICATIONS

INVESTIGATOR

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THE PROJECT

The existence of carbon nanotubes, which are carbon fibers at the nanoscale, was not known until the discovery of carbon nanotubes (CNTs) by Japan scientist Iijima in 1991. Since then, the research communities paid more attention to the fundamental properties of CNTs and found that CNTs have outstanding physical, chemical, electrical and mechanical properties.

CNTs are light-weight (one-sixth of the weight of steel) have very high tensile strength (1000 times that of the high carbon steel), high current densities (metallic nanotubes have current densities more than 1000 times than the copper and silver), good thermal conductivity (10 times that of copper) and are stable at 2800⁰ C. Because of these excellent properties, research is further intensified to find the potential applications in wide variety of science and engineering fields, such as in semiconductor devices, solar cells, high strength-low weight composites, to name a few.

We study the mechanical and electronic properties of carbon nanotubes using the atomistic simulations. The methods used here are *ab-initio*, tight-binding, molecular dynamics, continuum and hybrid by combining any of these methods.

In-house simulation code was developed and is capable of handling verity of problems related to carbon nanotubes and nanostructures.

Some of the studies from our simulations are (a) prediction of elastic properties of CNTs and its composites, (b) the behaviour of carbon nanotubes with temperature (thermal stability), (c) behaviour of CNTs under stretching, bending, and twisting, (d) fluid flow measurement of fluid conveying CNTs (Figure 1), (e) simulations for studying the flow behaviour of fluids inside the CNTs, (f) vibration behaviour of CNTs as a function of length and diameter (Figure 2), and other analysis of CNTs related nanostructures (Figure 3).

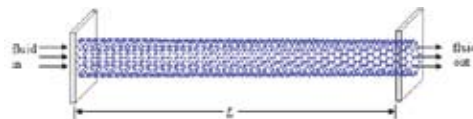


Fig.1 Schematic diagram of fluid conveying single walled carbon nanotube

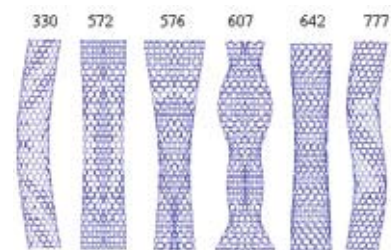


Fig.2 Natural frequencies (GHz) and vibration modes of single walled carbon nanotube

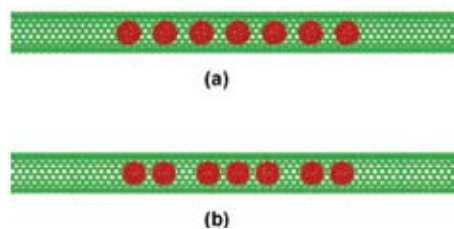


Fig.3 Clustering of encapsulated C60 molecules in carbon nanotube (a) initial structure (b) equilibrium states of C60 molecules after clustering.

SYSTEMS

SYSTEMS

IHPC has identified several research areas which have the potential to give rise to a broader set of technological innovations.

In this section, we highlight some of our work in interrogating challenging problems. Some of the areas highlighted are new opportunities for technological innovations, products and processes.

- Organsystems – Computational Otorhinolaryngology
- Computational Cancer Mechanics
- Thin Film Mechanics
- Multiphase/Interfacial Flow Dynamics
- Photonics
- Digital Modelling

Representative Publications

Liu S.Z., Luo X.Y., Lee H.P., and Lu C. "Snoring source identification and snoring noise prediction" *Journal of Biomechanics* **40** (4) 861-870 (2007)

SYSTEMS

ORGANSYSTEMS - COMPUTATIONAL OTORHINOLARYNGOLOGY

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THE PROJECT

IHPC's contribution to medical technology and bioengineering related research arises from our expertise in Computational Science and Engineering. The technology expertise and research areas can be broadly categorised as:

- Digital Modelling to build and reconstruct 3D models.
- Numerical Simulation to solve the related science and engineering problems. For example, flow analysis, fluid structural interaction, motion, and stress strain analysis.
- Visualisation and Data Mining to analyse the results and to bring the model to life.

For Digital Modelling, the expertise and research areas cover rapid construction of simulation models to achieve fast turnaround time, maximizing resources by digitally "recycling" simulation models, and provisioning of bio-models repository.

For Numerical Simulations, the research involves the integration of geometrical modelling to physical modelling and the applications of computational science and engineering to analyze and to predict the performance or behaviours.

For Visualisation and Data Mining, our work covers the development of algorithms and methodology for the analysis and visualisation of complex and large scale systems or data.

The current focus of the Organsystems@IHPC research program is on the computational modelling of geometrical configuration on human nose and its related physiologic functions in health and disease.

The nose is a natural and physiological respiratory passageway with approximately 10,000-20,000 liters of air moving through it daily on their way to the lungs. It has important physiological functions of conditioning and filtering inspired air, as well as immune defence function as the nasal mucosa is the first site of interaction between the host tissue and foreign invaders (i.e. bacteria, allergens and etc).

On the other hand, nasal obstruction, one of the most common symptoms, is difficult to quantify by clinical examination with the available techniques in clinical practice. Moreover, consequence or impairment of human airway physiology caused by nasal obstruction remains unclear.

The aim of this study is to establish a computational model of human nose and to investigate geometrical configuration of human nose in health and disease, and their impact on nasal airflow and its related physiologic functions.

The results of this study will provide insight into the physiologic functions of the nasal airway and nasal airflow, which is important in understanding the patho-physiological consequence of nasal obstruction. It will also be beneficial in medical teaching and in the potential development of new instrument for objective assessment of nasal airway and its related functions in clinical practice.

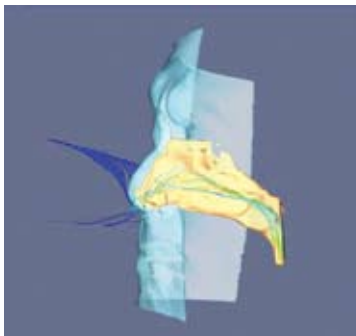


Fig.1 Airflow simulation of the nasal cavity



Fig.2 Simulation of the space under the nostril

SYSTEMS

COMPUTATIONAL CANCER MECHANICS

INVESTIGATOR

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THE PROJECT

Our current research focus is computational cancer mechanics. We use modelling and simulation to aid in the better understanding of the mechanical aspects of the cancer disease during its progression.

Cancer cells can break away from a tumor, penetrate into the circulatory and lymphatic systems and grow in a distant part of the body (see Figure 1). To do so, cancer cells have to degrade the proteins of the extracellular matrix, migrate through it, deform and squeeze through the endothelial layer of the capillaries before getting carried over large distances through the bloodstream. After traveling down the bloodstream, it will adhere to the endothelium, squeeze through it, and escape from the capillaries to proliferate to form a metastasis at a new site.

We want to model the deformation and migration of cells during metastasis. For example, we show in Figure 2 how a cell deforms and squeezes through a constriction, which could be a gap in the vascular endothelium. Knowledge of this mechanical process, such as the speed of migration, degree of deformation, etc., may be useful to cancer biologists in understanding how rapidly a metastasis spreads, and to bioengineers in designing diagnostic tools to detect cancer cells.

We are also working closely with experimentalists to validate our computational predictions. For example, we are currently collaborating with the group of Prof. Subra Suresh at the Massachusetts Institute of Technology to quantitatively measure the deformation and migration of cells in constricted microchannels.

Future research directions of the team will include the rearrangement of the cytoskeleton during cancer cell migration, the dynamics of the adhesion molecules on the cell membrane during migration, and the growth and vascularisation of a tumor.

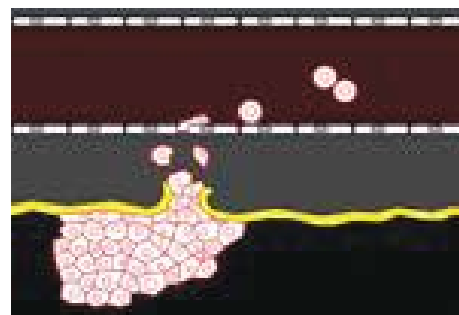


Fig.1 Steps in cancer metastasis. Cells deform and migrate to seed a secondary tumor at a distant part of the body. Understanding cell deformation and migration is a critical component of this process.

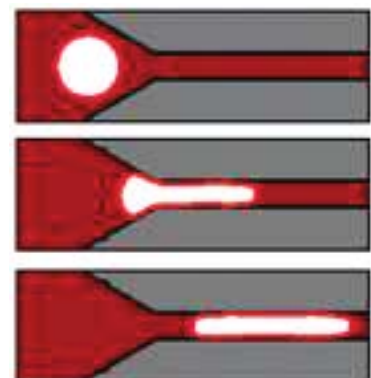


Fig.2 Simulation showing how a cell deforms as it squeezes through a constriction, which could be a gap in the vascular endothelium. Inside the constriction, the cell undergoes very large deformation and becomes "pancake"-shaped.

Representative Publications

Koh C.T., Liu Z.J., Khang D.Y., Song J., Lu C., Huang Y., Rogers J.A. and Koh CG, *Applied Physics Letters* **91** 133113 (2007)

SYSTEMS

THIN FILM MECHANICS

INVESTIGATOR

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THE PROJECT

Functional, stretchable and bendable electronics could be used in applications such as sensors and drive electronics for integration into artificial muscles or biological tissues, structural monitors wrapped around aircraft wings, and conformable skins for integrated robotic sensors.

In collaboration with researchers from the University of Illinois at Urbana-Champaign, IHPC is studying the unique mechanical characteristics of fully stretchable single-crystal silicon with micron-sized, wave-like geometries. We envisage that this material can be used to build high-performance electronic devices on rubber substrates, as the coupling of strain to electronic and optical properties might provide opportunities to design device structures that exploit the mechanically tunable and periodic variations in strain to achieve unusual responses.

To create the stretchable silicon, one method is the integration of thin films of high quality electronic materials (e.g. silicon) with elastomeric substrates for stretchable electronics (Figure 1). The first step involves fabrication of thin elements of single-crystal Si or completed integrated devices (transistors, diodes, etc) by conventional lithographic processing, followed by etching of the top Si and SiO₂ layers of a silicon-on-insulator wafer.

After these procedures, the thin film structures are supported by, but not bonded to, the underlying wafer. Contacting a prestrained, compliant substrate (e.g. PDMS) to the thin film leads to bonding between these materials. Peeling back the substrate, with the film bonded to its surface, and then releasing the prestrain, causes the substrate to relax back to its unstrained state. This relaxation leads to the spontaneous formation of well-controlled, highly periodic, stretchable wave structures in the thin film and near surface region of the substrate.

Our work in this area focuses on the prediction of the changes in amplitude and wavelength of the wrinkled wave through theoretical and numerical models (FEM) for buckling of thin films on compliant substrates well (Figure 2).

We also found that the numerical simulations could represent the regions of the films that lie near the edges. In these regions, the amplitudes of the waves decrease gradually to zero at the edge. This edge effect can be seen clearly in atomic force microscope and FEM simulation (Figure 2).

Such results might provide useful design guidelines in the applications of stretchable electronics. For example, well-placed edges can lead to flat regions in a larger scale buckled system where, for example, planarity is required for efficient photodetection or other functions. These and other possibilities appear to be interesting topics for further study.

Another possible application of stretchable silicon is in the fabrication of plastic electronics. Our interest in this facet of stretchable silicon research is in understanding the complex coupling between continuum mechanics and atomistic theories.

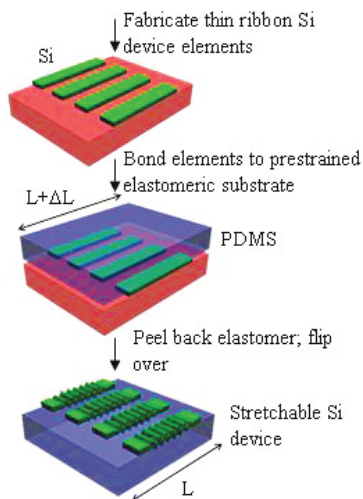


Fig.1 Schematically illustrates procedure of fabrication of stretchable silicon system

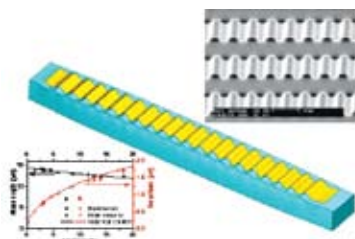


Fig.2 Experimental and simulated wrinkling silicon system.

Representative Publications

Klaseboer E., Khoo B.C. and Hung K.C. "Dynamics of an oscillating bubble near a floating structure" *Journal of Fluids and Structures* **21** 395-412 (2005)

Hua J.S. and Lou J. "Numerical simulation of bubble rising in viscouliquid" *Journal of Computational Physic* **222** (2007)

Ong W.L., Hua J.S., Zhang B.L. and Yobas L. et al. "Experimental and computational analysis of droplet formation in a high-performance flow-focusing geometry" *Sensor and Actuators: A. Physical* **138** 203-212 (2007)

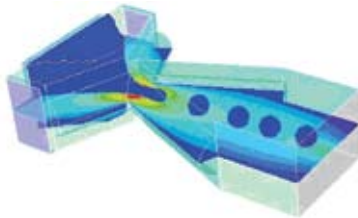


Fig.1 Microdroplet (~20 μm in diameter) formation in a flow focusing microfluidic device.

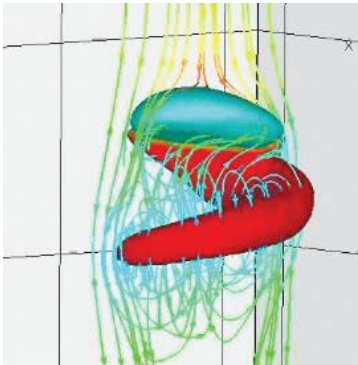


Fig.2 Detailed flow and wake structure after a spirally rising gas bubble in viscous liquid. The blue surface represents the bubble, and the red spiral surface is the wake

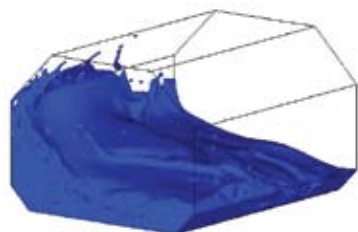


Fig.3 The oscillation of a free surface of sloshing liquid in a tank.

SYSTEMS

MULTIPHASE/INTERFACIAL FLOW DYNAMICS

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THE PROJECT

Multiphase fluid systems, involving liquid droplets, gas bubbles and free gas-liquid interfaces, can be encountered widely in nature (sea wave, rain drops), but also in many industrial (bubbly reactor, ink jet printing, spraying) and biological applications (BioMEMS, capsules). In many traditional engineering applications, the dynamics of dispersing bubbles / droplets into another liquid is commonly used to enhance heat and mass transfer or chemical reactions. The dynamics of super large under water explosion bubbles may significantly affect the structure of ships and submarines (Klaseboer et al, 2005).

With the recent development of micro fabrication technology, droplet-based micro-fluidic devices are becoming one of the most promising technologies for BioMEMS application (as shown in Figure 1). Micro-droplets have been used as a micro-container to encapsulate and transport chemical reactant in small volume and high concentration, and to host the reactions. To support applications of multiphase flow dynamics in such wide ranges of applications, a comprehensive understanding of multiphase flow physics is essential.

The fluid physics of such multiphase flows in association with bubbles, droplets and interfacial dynamics is, however, still not well understood, partly because of experimental difficulties in measuring and visualising such complex flow dynamics and phenomena, and theoretical challenges in analyzing such strongly coupled and non-linear systems. Numerical simulations have therefore provided a good alternative and can even lead to an extension of the physical understanding of the phenomena involved.

We focus on developing new algorithms for multiphase flow modelling and simulation, and exploring the flow physics underlying the complex multiphase flows (as shown Figure 2). Currently, a number of special methods of multiphase flow, such as front tracking method, Lattice Boltzmann method, level set method, boundary integral method, have been developed. These methods help us to explore bubble/droplet dynamics and physics in a wide range of applications. In addition, commercial software tools have also been applied to solve some large scale engineering multiphase flow problems as shown in Figure 3.

Representative Publications

Lim S.T., Ang Y.L., Png C.E. and Ong E.A. "Singlemode, Polarization-independent submicron silicon waveguides based on geometrical adjustments" *Optics Express* **15(18)** 11061-11072 (2007)

Png C.E., Lim S.T., Li E.P. and Reed G.T. "Tunable and sensitive biophotonic waveguides based on photonic-bandgap microcavities" *IEEE Transactions on Nanotechnology*, **5(5)** 478-483 (2006)

Png C.E., Chan C.P., Lim S.T. and Reed G.T. "Optical Phase Modulators for MHz and GHz modulation in Silicon-On-Insulator (SOI)" *IEEE J. of Lightwave Tech.* **22** 1573-1582 (2004)

SYSTEMS

PHOTONICS

INVESTIGATORS

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THE PROJECT

Increasingly smaller and faster semiconductor circuitry has fuelled an information technology boom over the past four decades, producing cheaper and more powerful computing devices that have boosted virtually every aspect of our economy. But fundamental limits imposed by the laws of physics threaten to halt continued miniaturisation, clouding the future of silicon-based semiconductors. With trillion-dollar investment each year in silicon fabrication technology, silicon is here to stay. This current situation encouraged scientists and engineers to find solutions to improve the devices performance. One alternative solution is silicon photonics, which utilise photons instead of electrons for data transfer.

At IHPC, we have successfully contributed to a number of key aspects in the field of Silicon Photonics research. For example, we have studied the critical aspects of single-mode and zero birefringence in nano-scale rib and strip optical waveguides at sub-micrometre scales, down to the very limit of waveguiding support at 220 nm. This is the first full mapping exercise of such waveguides and the results were published in *Optics Express* in September 2007. We have also experimentally demonstrated the first flat-top response in silicon arrayed waveguide gratings – a key component for multiplexing and demultiplexing of optical signals in a large network. A few years back, our team member has successfully predicted the first operating speed at 1 GHz silicon optical modulator, which was awarded a prestigious Royal Academy of Engineering Prize in the U.K. The ability to reach such a speed was verified experimentally by Intel scientists a year later and was reported in *Nature*. Since then, work in this area at IHPC, along with collaboration with Surrey University, U.K., has resulted in prediction of silicon optical modulators operating at 40 GHz, consequently, we predicted the speed of plasma-based silicon modulators to be approaching 100 GHz in 2006.

We also addressed the opportunity of mass adoption of photonic waveguides especially for sensing applications using multiple arrays. To achieve deployment for mass arrays, the device must be highly sensitive, ability to be miniaturised, mechanically stable, and immune to electromagnetic interference, which can be realised using photonic bandgap structures. Such device could be featured into a "go/no-go" biosensing instrumentation for initial investigation. On top of these considerations, the device must be cost-effective to manufacture and this means that the waveguides have to be easily fabricated. We improved the attractiveness of this passive waveguide by introducing active switching elements capable of power reduction by five-orders of magnitude compared to conventional optical waveguides. These results were reported in the scientific literature including *IEEE Transactions on Nanotechnology* and *IEEE Journal of Selected Topics in Quantum Electronics* in 2006. Another resultant of this work was in the form of an intellectual property consisting of a multiple sensing device based on nano-cavity with wide fabrication tolerances and increased in transmission and quality factor.

Due to our expertise in the area of active devices, we were also engaged by industry to study novel structures which require novel methodologies in 3-D optical and electrical simulations for chromatic dispersion compensators (CDC) – a key component for optical networks. The next generation of research in IHPC will be focusing on short distance communication such as on-chip interconnects, and chip-chip interconnects. Collaboration with groups from both academia and industries is highly anticipated.

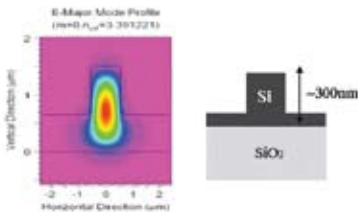


Fig.1 Mode studies on Nano-silicon waveguides

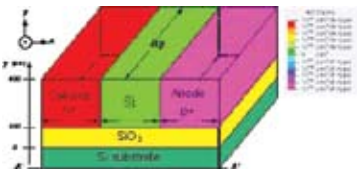


Fig.2 The active switching optical diode in the microcavity region

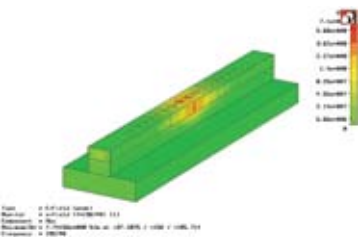


Fig.3 1-D photonic bandgap nano-cavity

Representative Publications

Chong C.S., Lee H.P. and Kumar A.S. "Genetic algorithms in mesh optimization for visualisation and finite element models" *Neural Computing and Applications* **15 (3-4)**, 366-372 (2006)

Chong C.S., Lee H.P. and Kumar A.S. "Automatic hole repairing for cranioplasty using Bezier surface approximation" *Journal of Craniofacial Surgery* **17 (2)** 344-352 (2006)

SYSTEMS

DIGITAL MODELLING

INVESTIGATORS

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THE PROJECT

The Digital Modelling and Visualisation Team engages in R&D activities to bring the science of computational geometry and modelling to the domain of computational science and engineering. In general, digital modelling research in IHPC comprises of five key components, namely reconstruction, restoration & repair, reduction & refinement, recycling and repository. These five components also represent the value chain of mesh creation and utilisation, from the process of creating the mesh from input data, to mesh manipulation, and finally to the reusability of the meshes.

In terms of reconstruction, the capabilities include the reconstruction of meshes from a wide range of raw input, which includes point cloud data, CAD data, facial images, medical images from CT/MRI scans and geographical information systems data. While the reconstruction techniques are based on robust mathematical foundation, the quality of the reconstructed meshes is limited by the input data itself. It is inevitable that missing data might result in incomplete or problematic meshes and an additional procedure of mesh restoration & repair is usually required. Moreover, using an in-house meshing package that is developed in IHPC, called the Virtual Geometry kernel, the resolution of the meshes has been adaptively modified (refined or reduced) to suit different applications.

The notion of digital recycling is to be able to rapidly transform an existing mesh which sufficiently matches the desired model so that the time-consuming process of meshing from scratch is avoided. Models which have been created can then be provision in a repository for storage, retrieval and reuse. Such a framework will allow researchers to conduct their work and simulation more efficiently.

With increased understanding in the science of digital modelling for static 3D meshes, we have also transited to managing and processing dynamic meshes. This exciting area of geometrical modelling allows the application of digital modelling in complex simulation, as well as in other fields, like the biomedical sciences.



Fig.1 An Overview of the various capabilities in the Digital Modelling Team.



Fig.2 Automatic Mesh Healing and Restoration for Simulation



APPLICATIONS



APPLICATIONS

IHPC is constantly on the pulse of developments in emerging applications of areas such as nanotechnology, wireless communications and clean energy, to name a few.

Leveraging on our broad skill-base, we are well-placed to conduct research into a myriad of exciting nascent technologies that could improve our quality of life in the future. Our main aim in this concern is in the establishment of enabling capabilities and platforms to facilitate the development of new applications.

- Bubble Dynamics
- Fluid Flow in Microenvironments
- Computational Vibro-Acoustics Modelling and Simulation for Virtual Product Development
- Systems on Package
- Wireless Body-Area Network
- Shared Services
- Clean Energy

Representative Publications

Turangan C.K., Ong G.P., Klaseboer E. and Khoo B.C.
"Experimental and numerical study of transient bubble-elastic membrane interaction" *Journal of Applied Physics* **100** 054910 (2006)

Fong S.W., Klaseboer E., Turangan C.K., Khoo B.C. and Hung B.C.
"Numerical analysis of a gas bubble near bio-materials in an ultrasound field" *Ultrasound in Med. & Biol.* **(32)** 925-942 (2006)

APPLICATIONS

BUBBLE DYNAMICS

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THE PROJECT

Bubbles can be found in many environmental, industrial and biomedical related areas. The bubbles studied here are pockets of vapour or air in water (not to be confused with soap bubbles!). The study of bubbles can be divided in two main areas: rising bubbles (such as in a fish tank) and oscillating bubbles (such as in cavitating ship propellers).

The main focus of the study is on oscillating bubbles, which show some very interesting phenomena. Due to the compressibility of the contents of the bubble, the volume of the bubble can change with time. Often, when a bubble collapses, a very high speed jet (100 m/s or higher) is observed. This jet can destroy nearby material. The smaller the size of the bubble, the faster it oscillates: for example, when disturbed, a 1 mm bubble oscillates in only 0.1 millisecond. Very small bubbles can not be detected anymore unless very high speed cameras are used. Therefore numerical simulations are the ideal tool to study these bubbles.

IHPC has developed its own in-house numerical code based on the so-called boundary element method to simulate oscillating and collapsing bubbles. It has been used for a variety of purposes ranging from underwater explosions to several bio-medical applications such as kidney stone removal, dental applications, eye surgery, etc. In Figure 1 a numerical simulation is shown of a bubble oscillating near cornea like material. The study of microbubbles (small pockets of air, coated with a membrane) is of special interest and its interaction with pressure perturbations (such as shock waves or high intensity pulsed ultrasound) might very well be used in the future to treat a variety of diseases such as cancer (by destroying the tissue with a collapsing bubble).

Other, non-medical applications are also studied, such as ultrasonic cleaning (where jets from collapsing micro-bubbles are believed to do the cleaning).

Another area is micropumps, where the jet of a collapsing bubble pumps small amount of liquid through a plate with a hole (see Figure 2). A patent was granted to IHPC/NUS based on this principle.

Experiments were performed in NUS and other collaborating universities around the world in collaboration with NUS, NTU, Duke University, Twente University (The Netherlands), etc. An example of such an experiment can be seen in Figure 2.

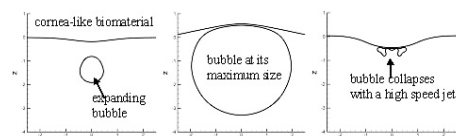


Fig.1 Bubble shapes at the second period of oscillation of a bubble at 1.5 initial bubble radius, R_0 , away from a cornea-like biomaterial (whose surface is represented by the line on top of the bubble). The bubble interacts with a strong ultrasound field by expanding initially (left most picture) and then obtains its maximum size (center picture), pushing back the cornea tissue. Lastly it collapses with a high speed jet of about 100 m/s towards the cornea (right most picture). As the cornea tissue is also moving towards the collapsed bubble, the strong jet might cause severe damage to the cornea tissue.

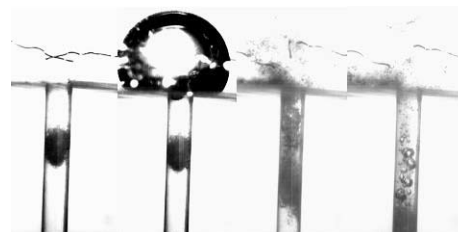


Fig.2 A spark bubble of maximum radius, $R_{max} = 3.7$ mm is generated 2.0 mm above a hole of 1.8 mm in an acrylic block. Initially the center of the fiber ball (wetted weight = 4.6 mg) is located 4.1 mm from the tube top. Then it is pushed 5.1 mm down the tube finally. The pictures from left to right are taken at 0, 0.8, 2.8, and 6.6 ms respectively. The two horizontal bars indicate the top and bottom of the fiber ball. This principle (using the jet of a collapsing bubble), can also be used for micro-pump applications.

Representative Publications

Pan L.S., Xu D., Lou J. and Yao Q.
"A Generalized Heat Conduction Model in Rarefied Gas" *Europhysics Letters* **73 (6)** 846-850 (2006)

Hua J.S., Zhang B.L. and Lou J.
"Numerical simulation of micro-droplet formation in micro-channel with co-flowing immiscible liquid" *AIChE Journal* **53 (10)** 2534-2548 (2007)

APPLICATIONS

FLUID FLOW IN MICROENVIRONMENTS

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THE PROJECT

Microfluidics is a multidisciplinary field comprising physics, chemistry, electronics, material, engineering and biotechnology that studies the behaviour of fluids at the microscale, that is, fluids at volumes thousands of times smaller than a common droplet. It also concerns the design of systems in which such small volumes of fluids will be used, such as in a lab-on-a-chip device. Microfluidics has found various important applications like new drug discovery, micro-droplet/particle processing, micro-reactor, and micro-sensors.

Combining IHPC's unique multidisciplinary expertise, we have investigated the microfluidic phenomena by multiscale computational model simulations. We have developed in-house codes ranging from modified continuum model, Direct Simulation Monte Carlo, to particle dynamics models. The developed models have been successfully applied to:

- rarefied gas flow in microchannel;
- 3-dimensional micropumps/valves with full fluid/structure interaction;
- droplet formation in micro-device;
- suspension flow in microfluidics;
- electromorphology cell traps;
- micro-needle analysis

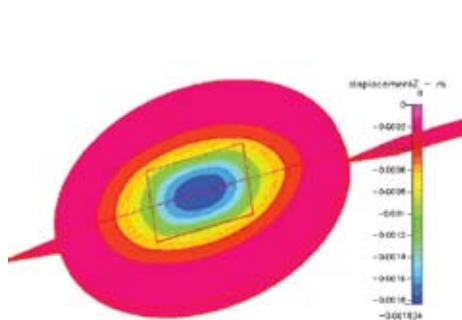


Fig.1 Deformation of the membrane surface of a piezoelectric micro-pump.

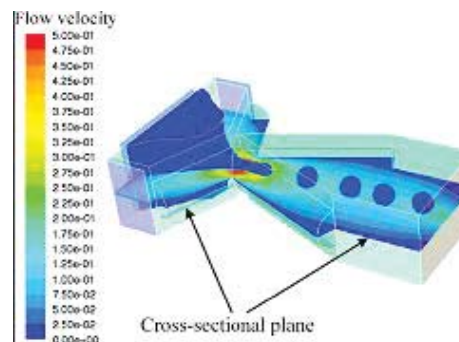


Fig.2 Generation of microdroplet with disperse shear flow in micro nozzle.

Representative Publications

Cai C., Zheng H., Hung K.C. and Zhang Z.J. "Vibration analysis of a beam with ACLD patch" *Smart Material and Structures* **15**, 147-156 (2006)

Zheng H., Tan X.M. and Cai C. "Damping analysis of beams covered with multiple PCLD patches" *International Journal of Mechanical Science* **48** 1371-1383 (2006)

Cai C., Cheng M. and Hung K.C. "High Performance Muffler" US Patent Number: US 6,892,853

APPLICATIONS

COMPUTATIONAL VIBRO-ACOUSTIC MODELLING AND SIMULATION FOR VIRTUAL PRODUCT DEVELOPMENT

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THE PROJECT

Companies today are facing ever more challenges in developing new products due to an increasingly competitive market place. To shorten the development cycle from concept design to launching high-quality products to the market, and to reduce the cost of physical prototypes involved in the development cycle, a company has to rely increasingly on computational science and engineering based virtual product development techniques.

One important consideration in the development cycle is vibration characteristics and acoustic noise level. Vibro-acoustic modelling and simulation technology has become a critical element of the competitive strategy of virtual product development. The acoustic noise levels and sound quality can be predicted early in the design of new products with appropriate accuracy by utilising vibro-acoustic modelling and simulation techniques integrated in the development circle; and an understanding of the impact of design modification on the acoustic noise level can be achieved much faster than building and testing physical prototypes.

The vibro-acoustic modelling and simulation study at IHPC initially focused on the development of capability in the prediction of structural vibration and acoustics, such as cabin noise level prediction and exterior acoustic signature simulation of underwater and ground vehicles at the early product design stage. The focus of the study was then concerned with the enhancement of the developed capability in vibro-acoustic modelling and simulation, and also on simulation-based development of effective noise and vibration control measures such as smart damping, resilient mounts and active coating. This work has been done through conducting up-stream and application research in collaboration with prestigious academic organisations and engineering companies.

Some of our recent developments in the area include:

- Acoustic noise modelling & sound quality analysis of hard disk drives
- Track noise modelling & prediction
- Virtual development of a high-performance exhaust muffler
- Vibro-acoustic modelling of smart panels for active noise mitigation of vehicles.

The simulation-based muffler design project, for example, resulted in the development of a successful methodology to model reactive and dissipative mufflers with bulk sound absorbing materials and perforated tubes. This has been a challenge in the community because volume and weight constraints of designing a muffler for reduction of the exhaust noise from an engine have become ever more stringent.

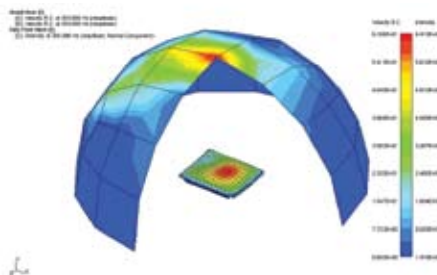


Fig.1 Vibro-acoustic modelling of a HDD

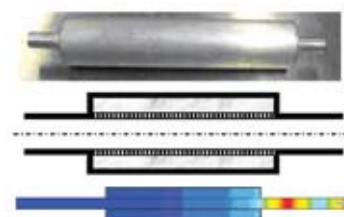


Fig.2 Simulation-based muffler design

Representative Publications

Wei X.C., Li E.P., Liu E.X., and Oo Z.Z. "Emission and Susceptibility Modelling of Power-ground Plane with Finite-size by using a Novel Hybrid Integral Equation Method" to appear in IEEE Trans. Adv. Packag.

Oo Z.Z., Liu E.X., Li E.P. and Wei X.C., et al "A Systematic Semi-Analytical Approach for System-Level Electrical Modelling of Electronic Packages with Large Number of Vias" to appear in IEEE Trans. Adv. Packag.

APPLICATIONS

SYSTEMS ON PACKAGE

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THE PROJECT

Moore's law predicts the doubling of transistors on a chip every 18 months. But it is beginning to reach its limit in miniaturisation. Fortunately, this bottleneck can be alleviated by system integration such as System-in-Package (SIP) and System-on-Package (SOP). However, design and simulation tools are yet to be developed for future system integration. Novel electrical modelling technologies are highly demanded to tackle the challenges posed by the silicon complexity and system complexity of nano-scale integrated circuits (ICs) integration and packaging.

Our research team is currently working on the simulation for system-level packaging. The objective of the project is to develop efficient yet accurate algorithms and methodologies for modelling and simulation of advanced IC packaging. It is devoted to address the system-level modelling and analyses of IC packages to ensure signal integrity, power integrity and electromagnetic compatibility (EMC).

We are currently developing a novel technique for analysis of signal integrity, power integrity and EMI (electromagnetic interference) in the system-level packaging. The technique is able to address the electromagnetic coupling and wave interactions among a large number of vias in the presence of multiple power/ground planes. The scattering matrix method (SMM), coupled with a new boundary modelling technique that we developed, is a viable method for practical package modelling with multiple vias in a finite domain.

Furthermore, we will extend the current simulation techniques to perform chip-package co-simulation incorporating thermal and mechanical modelling capabilities. Mixed electrical-optical modelling and other emerging problems pertaining to future generations of IC and packages will also be addressed to meet the requirements of the future development in semiconductor industry.



Fig.1 A schematic view of an electronic package

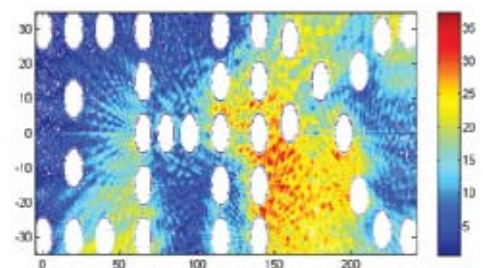


Fig.2 Coupling among vias in a package

Representative Publications

Lim H.B., Baumann D., Koh R., Cai J., Li E.P. and Lu Y "Antennae Polarization for Effective Transmission of UWB Signal around Human Body" Intern. Conf. on UWB (ICUWB) (2007) Singapore

Fumeaux C., Baumann D., Sankaran K., Krohne K., Li E.P., and Vahldieck R. "The Finite-Volume Time-Domain Method for 3-D Solutions of Maxwell's Equations in Complex Geometries: A Review" Proceedings of the European Microwave Association (EuMA) **3** 136-146 (2007)



Fig.1 Model of two disc-cone antennas placed on a human arm.

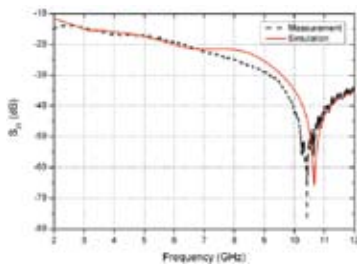


Fig.2 Comparison between measurement (black dashed line) and simulation (red solid line) of the transmission coefficient S_{21} of two disc-cone antennas placed on a human arm at a distance of 5 cm.

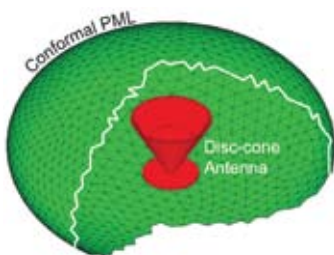


Fig.3 Conformal PML boundary surrounding the model of a disc-cone antenna used in FDTD.

APPLICATIONS

WIRELESS BODY-AREA NETWORK

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THE PROJECT

One of the most promising applications of WBAN is wearable health care for remote monitoring of a patient's vital signs without obstructing the patient's everyday life. Commonly, a WBAN consists of several sensors and antennas distributed over the human body serving as a communication network.

The ultrawideband (UWB) technology is proposed for communication within a WBAN because of its various advantages over narrowband systems, e.g. low transmit power and high bandwidth for fast information transmission.

At IHPC, in collaboration with the Institute for Infocomm Research (I²R), A*STAR, and the Laboratory for Electromagnetic Fields and Microwave Electronics (IFH), ETH Zurich, Switzerland, the characteristics of UWB signal transmission in close proximity to the human body is investigated. The influence of the body composition, such as shape or multi-layered tissue structure is determined in order to provide a design reference for a WBAN system. As depicted in Figure 1, disc-cone antennas are used as test antennas in the initial investigation. However, this type of antennas is rather bulky and hence will be replaced at a later stage of the project.

The strategy for the investigation is twofold: 1) The employment of commercial software allows quick characterisation of the communication system. As shown in Figure 2, measurements on a human arm are compared to simulations using CST Microwave Studio® with a good agreement. 2) The development of an in-house code based on the Finite-Volume Time-Domain (FVTD) method enables custom-tailored analysis of highly specialised problems. The FVTD method is applied in an unstructured mesh which is advantageously exploited especially for complex geometries such as a WBAN. To further enhance the FVTD's strengths, a conformal formulation of the Perfectly Matched Layer (PML) absorbing boundary condition is investigated, enabling the use of an arbitrarily shaped boundary as depicted in Figure 3.

APPLICATIONS

SHARED SERVICES

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THE PROJECT

In November 2006, IHPC and HP Labs embarked upon a three year collaboration to provide "IT/HPC as a Service". The focus of the effort is to research and pilot technologies to provide IT services in an automated, repeatable and cost-effective manner. These technologies will benefit IT departments in large enterprises and third-party IT service providers as well as systems companies who provide the technologies to them. In addition, these are services that can capture and codify the essence of marketplace business such as service level agreement (SLA) negotiation and management, and economics.

The output of the collaboration is expected to provide innovative solutions to barriers that limit the construction and use of shared services environments within a marketplace; pilot those solutions with customers within Fusionopolis and Singapore; and encourage the adoption / commercialisation of those solutions.

The research is performed in the context of a *shared services platform* (see Figure 1) – a set of services, capabilities, software, tools and processes that are designed to support such use cases. The platform will be based on service oriented architecture (SOA) principles; it includes support for both high-performance computing (HPC) and enterprise uses. And it is constructed in a way that allows independent users, service providers and research teams to benefit from it.

Research challenges that are addressed include development of the SOA architecture necessary for the platform; modelling the various services such that they can be dynamically composed in a flexible and rapid manner; understanding the service-level requirements of the various stakeholders; and developing service-level mechanisms that allow the services (and the ecosystem they are part of) to adapt to changing needs and priorities.

The goal finally is to create a platform using a SOA architecture to enable real-time plug-n-play and mashup/composition of services. This requires formal definitions of services to be able to reason about correctness in composed services and service behaviour; decentralised definition and versioning of services to disaggregate model creation and maintenance; and the ability of evolve services and protocols.

The approach is to combine SOA with model-driven automation (MDA) where each service exposes a model of itself. The idea is to model both the service itself as well as the resources/entities managed by the service. The approach also dictates that all services use models for interaction and composition; and models are used for mediation, discovery, versioning, design configuration, etc by the SOA. This platform provides several advantages over traditional web services in that it provides mechanisms for formal validation of correctness of composed services and stronger "hooks" for extensibility, security, and introspection of services.

Building on top of the SOA architecture are various other research thrusts such as model validation, service level management, and economic considerations for the service ecosystem.

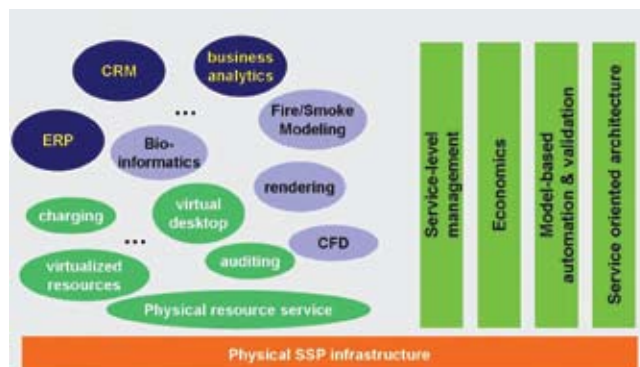


Fig.1 Shared Services Platform

APPLICATIONS

CLEAN ENERGY

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THE PROJECT

Fuel cell technology presents huge economical and environment potential for the next-generation power systems because it can offer great advantages over the conventional power-generating systems in terms of both the energy efficiency and the emission reduction. Besides that, the popularity of this renewable energy source is also highly motivated by the global fuel price increase. One of these fuel cells is the Proton Exchange Membrane Fuel Cell (PEMFC), which is a low temperature fuel cell. These fuel cells convert hydrogen or hydrocarbon fuels directly into electricity. It is highly versatile as it can be used for portable devices, vehicles, as well as stationary power plants.

In view of the huge potential industrial demand in this alternative energy source, IHPC has embarked on the computational modelling works on PEMFC since 2003. The fuel cell research works are highly multi-disciplinary, as it involves research community from mechanical, electrical, material science, mathematicians and physicians.

The core PEMFC research works comprises:

- i. membrane science
- ii. catalysts and electrochemistry
- iii. thermo-fluids and component design
- iv. system integration.

For IHPC modelling work, our effort is mainly focused on the third component, in which the researchers would carry out detailed modelling analysis to investigate the effect of transport phenomena (molecular diffusion, ion migration, convection), multi-phase physics (water management), heat transfer (performance stability) and fluid dynamics (flow channel design) on PEMFC performance.

The following PEMFC projects had been carried out in IHPC:

- 1) Modelling "Air-Breathing, Self-humidifying PEM Fuel Cell" to obtain polarisation curves for various channel designs for micro PEMFC using CFD simulations and validating with experimental results (in collaboration with SIMTech)
- 2) Optimizing flow distributors designs of to improve PEMFC performance (in collaboration with NUS)
- 3) Exploring potential mass transport enhancement in PEMFC through the concept of impinging jet (in collaboration with NUS)
- 4) Modelling "Dead End Anode and Self Breathing Cathode PEMFC" to study its performance (in collaboration with an industry partner)

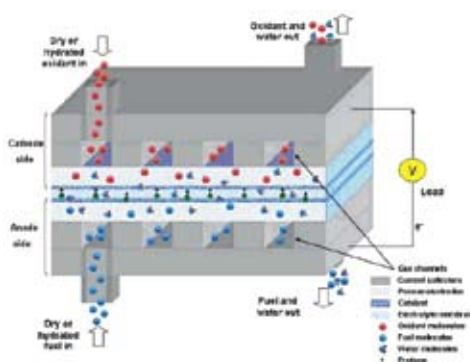


Fig.1 Schematic of a fuel cell

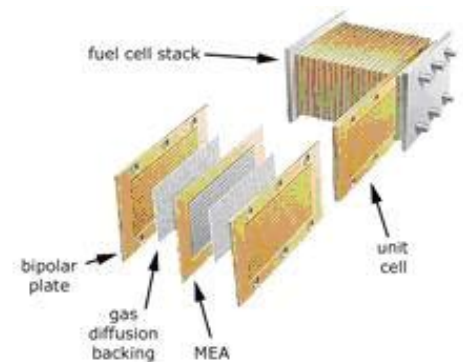


Fig.2 Schematic of a fuel cell stack

IHPC RESEARCH PROGRAMMES



IHPC RESEARCH PROGRAMMES

- Advanced Computing Programme
- Computational Materials Science and Engineering Programme
- Engineering Software and Applications Programme
- Large Scale Complex Systems Programme



ADVANCED COMPUTING PROGRAMME

The focus of the Advanced Computing Programme is in the development of technologies to address compute, data and graphics intensive applications in the science and engineering domains. Our researchers strive to establish end-to-end capabilities to enable research and industry communities in large-scale and globally distributed science and engineering activities.

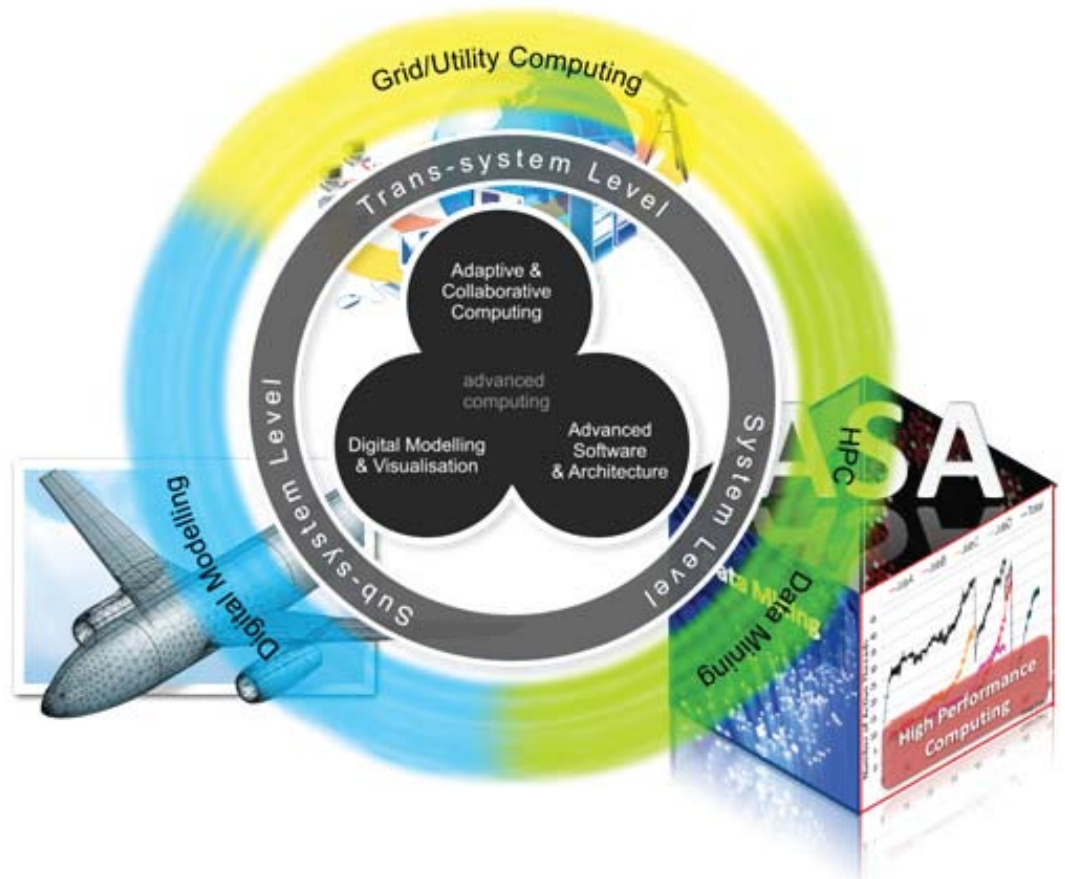
For compute-oriented problems, we exploit technologies in high performance and grid computing technologies. In tandem with helping to manage and understand large complex data, we also explore and utilise computational intelligence and visualisation strategies.

Our Research Teams

- Adaptive and Collaborative Computing
- Digital Modelling and Visualisation
- Advanced Software and Architecture

Our Research Capabilities

- Grid computing middleware & grid-enabling of applications
- HPC algorithms and application optimisation
- Digital modelling and Reconstruction
- Data mining for infectious diseases and environment control



COMPUTATIONAL MATERIALS SCIENCE AND ENGINEERING PROGRAMME

The mission of the Computational Materials Science and Engineering Programme is to predict, explore and understand the fundamental properties and structure of materials, and to develop new materials using novel computational approaches.

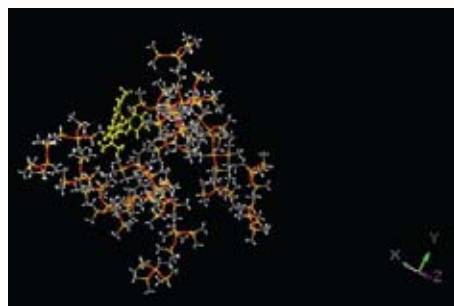
We perform basic materials science research such as atomistic modelling, molecular simulations, materials informatics to develop advanced electronics as well as green energy and materials. A unique set of APEX (Advanced Process Expert) data-mining techniques has also been applied to solve industrial problems.

Our Research Teams

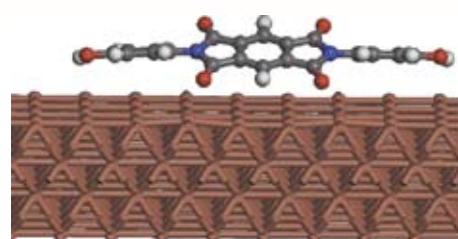
- Computational Chemistry
- Multiscale Modelling
- Solid State Electronics and Nanostructures

Our Research Capabilities

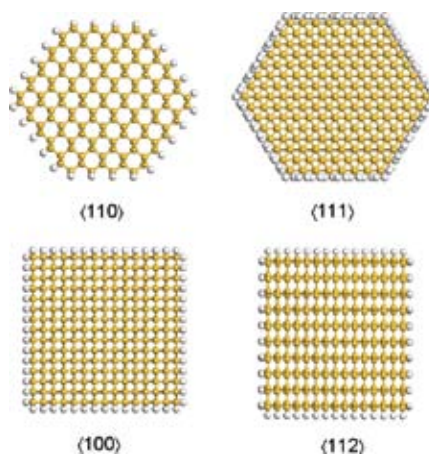
- Multiscale modelling
- Atomistic modelling
- Materials informatics
- Nanodevice simulation
- Chemical thermodynamics and kinetics modelling
- Process simulation
- Materials by design
- Alloy formulation
- Catalyst formulation
- Nanocomposite formulation
- Design of synthesis routes



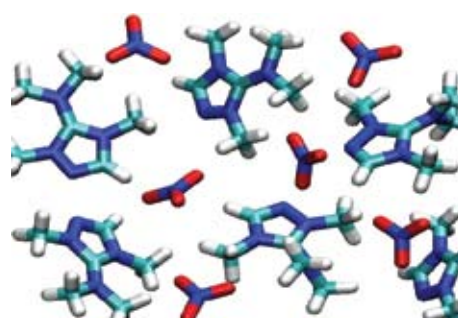
Perform MD Simulation to identify polymers and dyes that fit together



Metal-polymer interactions



Cross section of silicon nanowires



Simulation of structure, dynamics and energetics

ENGINEERING SOFTWARE AND APPLICATIONS PROGRAMME

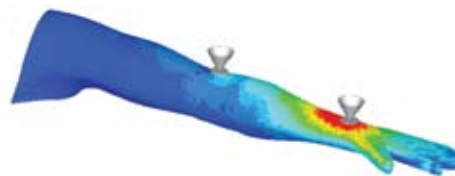
The Engineering Software and Applications Programme exploits the use of high performance computing technologies for key sectors such as electronic devices and systems. We mainly focus on the development of new electromagnetic simulation algorithm, the modelling and analysis of electromagnetic fields, Silicon photonic devices, plasmonics nano-structures and Silicon-based nano-electronics.

Our Research Teams

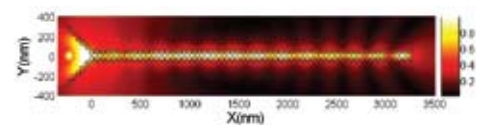
- Electronic Systems
- Engineering Software

Our Research Capabilities

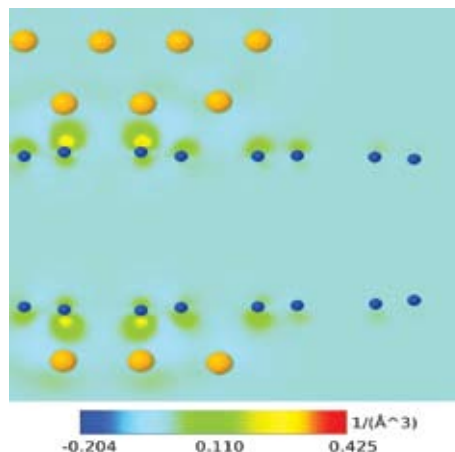
- Development of time- and frequency-domain electromagnetic numerical methods
- Computational techniques for electromagnetic wave propagation, EMC/EMI
- Nano-scale integrated circuit and the package integration simulation
- Optical and electrical simulations of Silicon photonic devices
- Modelling of plasmonics nano-structures
- Simulation of nano-scale electronics



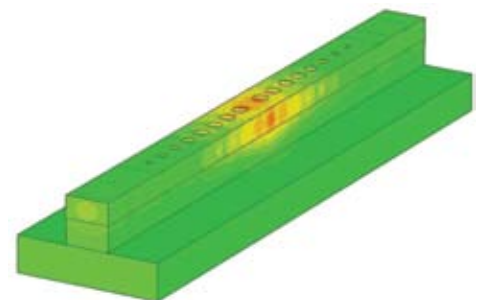
Surface current distribution on a human arm at 3 GHz



Near-field distribution of a double-chain metallic nanowire array at wavelength $\lambda = 600$ nm



Charge transfer between metal Al and Carbon atoms



E-field resonance of a 1-D photonic bandgap

LARGE SCALE COMPLEX SYSTEMS PROGRAMME

Large Scale Complex Systems research is driven by a desire to understand natural systems – systems that are inherently complex, governed by multiple physical regimes and that incorporate diverse theories. Our research directions are based on our current expertise and an interest in expanding our capabilities. There is a diverse range of science and engineering disciplines represented in the programme – mechanics, mathematics, physics and chemical engineering.

Our Research Teams

- Engineering Mechanics
- Computational Fluid Dynamics
- Heterogeneous Coupled Systems
- Biophysics

Our Research Capabilities

Large-Scale (Computational)

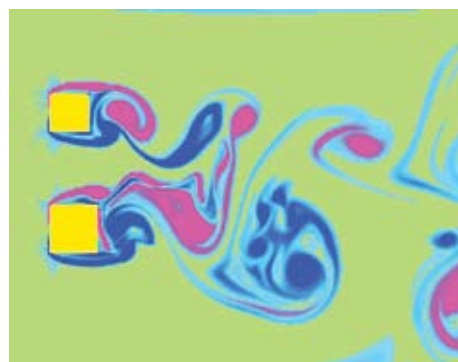
- Molecular dynamics simulation
- Bubble dynamics
- Air dispersion
- Vibration and acoustics
- Offshore engineering

Complexity (Mathematical)

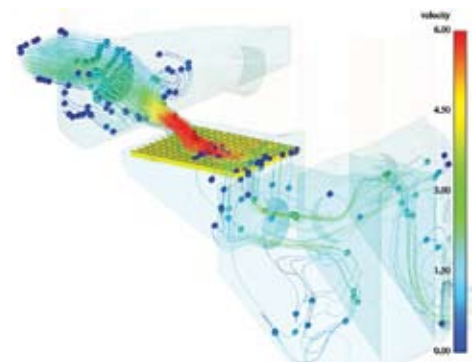
- Thin film mechanics
- Multiphase flow
- Multiscale modelling
- Turbulence
- Chaotic dynamics
- Nanomechanics

Multiphysics (Physical)

- Nucleation and Crystallisation
- Cell dynamics
- Fluid structure interaction



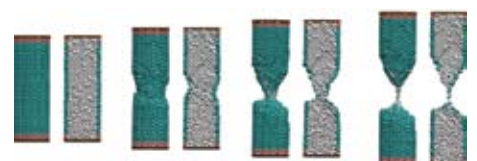
Simulation of fluid flowing around blocks



Simulation of flow of water pumped out from a shaft



Crystallisation process



Amorphisation in Metallic Nanorods



FY2007 SELECTED PUBLICATIONS

No	Title of Publication	Name of Journal	Date of Publication	Ist Author Name	Other Author Names	IHPC Research Programme
1	A Window-assisted Video Partitioning Strategy for Partitioning and Caching Video Streams in Distributed Multimedia Systems	Journal of Parallel and Distributed Computing (JPDC)	Vol. 67, Issue 6, pages 738-754, June 2007	Li X.R.	Veeravall B., and Prasanna V.K.	Advanced Computing
2	Modification of activated carbon by polyaniline for enhanced adsorption of aqueous arsenate	Industrial & Engineering Chemistry Research	Vol 46 (7), pages 2133-2140, Mar 28 2007	Yang L.	Wu S.N. and Chen J.P.	Computational Materials Science and Engineering
3	Adsorption of molecular oxygen on the walls of pristine and carbon-doped (5,5) Boron Nitride Nanotube: a spin polarized density functional study	Physical Review B	Vol. 75 page 245301, 2007	Zhang J.	Loh K.P., Zheng J.W., Sullivan M.B., and Wu P.	Computational Materials Science and Engineering
4	Large scale ab initio molecular dynamics simulations of hydrogen-induced degradation of Ta diffusion barriers in ultralow-k dielectric systems	Applied Physics Letters	Vol 90, page 032906, 2007	Dai L.	Tan V.B.C., Yang S.W., Wu P. and Chen X.T.	Computational Materials Science and Engineering
5	Proton interaction in phosphate adsorption onto goethite	Journal of Colloid and Interface Science	Vol 308(1), pages 40-48, Apr 2007	Zhong B.	Stanforth R. and Wu S.N.	Computational Materials Science and Engineering
6	Simulations on effects of granular morphology on single-electron and optical spectra of nano- and micro-crystalline AlN and diamond	Diamond and Related Materials	Vol 16 (4-7), pages 784-789, April-July 2007	Ligatchev V.	Ong K.P. and Wu P.	Computational Materials Science and Engineering
7	Nonequilibrium Green's function method for thermal transport in junctions	Physical Review E	Vol 75 (6), pages 1128-1128 Part, 1 Jun 2007	Wang J.S.	Zeng N., Wang J., and Gan C.K.	Computational Materials Science and Engineering
8	Magnetic Molybdenum Disulfide Nanosheet Films	Nano Letters	Vol 7 (8), pages 2370 -2376, 2007.	Zhang J.	Soon J.M., Loh K.P., Yin J.H., Ding J., Sullivan M.B. and Wu P	Computational Materials Science and Engineering
9	Understanding Nitrogen-induced effects on the performance of Ultra Low-K Dielectric Systems through Ab Initio Simulations	Surface Science	Volume 601, Issue 16, pages 3366-3371, 15 August 2007,	Dai L.	Tan V.B.C., Yang S.W., Wu P. and Chen X.T.	Computational Materials Science and Engineering
10	p-type conduction in unintentional carbon-doped ZnO thin films	Applied Physics Letters	91 (7), page 072101, Aug 13, 2007	Tan S.T.	Sun X. W., Yu Z. G., Wu P., Lo G. Q. and Kwong D. L.	Computational Materials Science and Engineering
11	Theoretical investigation of silicon nanowires: Methodology, geometry, surface modification, and electrical conductivity using a multiscale approach	Physical Review B	Vol 76, Article No. 155435, 2007	Ng M.-F.	Zhou L.P., Yang S.W., Sim L.Y., Tan V.B.C. and Wu P.	Computational Materials Science and Engineering
12	Electronic properties of A-site substituted lead zirconate titanate: Density functional calculations	Physical Review B	Vol 76, Article No. 125102, 2007	Zhang Z.	Wu P., Ong P.K., Lu L. and Shu C.	Computational Materials Science and Engineering
13	Two-dimensional space-charge-limited flows in a crossed-field gap	Applied Physics Letters	Vol. 90, page 141503 (2007), April 2007	Koh W.S.	Ang L.K.	Engineering Software and Applications
14	Analysis of Sub-Wavelength Light Propagation Through Long Double-Chain Nanowires with Funnel Feeding	Optics Express	Vol. 15, Iss. 7, April 2007	Chu H.S.	Ewe E.B., Li E.P. and Vahldeick R.	Engineering Software and Applications
15	AIM Analysis of Scattering & Radiation by Arbitrary Surface-Wire Configurations	IEEE Transactions on Antennas and Propagation	Vol. 55, No. 1, April 2007	Ewe W.B.	Li L.W., Chang C.S. and Xu J.P.	Engineering Software and Applications
16	Numerical dispersion analysis with an improved LOD-FDTD method	IEEE Microwave and Wireless Components Letters	17 (5): 319-321 MAY 2007	Li. E.P.	Ahmed I. and Vahldeick R.	Engineering Software and Applications
17	AIM Analysis of EM Scattering By Arbitrarily Shaped Mageodielectric	IEEE Transactions on Antennas and Propagation	vol. 55, no. 7, pages 2073-2079, Jul 2007	Ewe W.B.	Li E.P., Chu HS and Li L.W.	Engineering Software and Applications
18	Single mode, polarizationindependent submicron silicon waveguides based on geometrical adjustments	Optics Express	Vol. 15, No. 18, pages 11061-11072 Sep 2007	Lim S.T.	Png C.E., Ong E.A. and Ang Y.L.	Engineering Software and Applications
19	Numerical Simulation of Bubble Rising in Viscous Liquid	Journal of Computational Physics	Vol.222 (2), pages 769-795. Mar 20 2007	Hua J.S.	Lou J.	Large-Scale Complex Systems
20	Dynamic Simulation of a WWTP Operated at Low Dissolved Oxygen Condition by Integrating Activated Sludge Model and a Floc Model	Biochemical Engineering Journal	Vol.33, pages 217-227 February 2007	Wang C., Zeng Y.	Lou J. and Wu P.	Large-Scale Complex Systems
21	Designing Process Controller For A Continuous Bread Baking Process Based On CFD Modelling	Journal of Food Engineering	Vol.81, pages 523-534, March 2007	Wong S. Y.	Zhou W.B. and Hua J.S.	Large-Scale Complex Systems

No	Title of Publication	Name of Journal	Date of Publication	Ist Author Name	Other Author Names	IHPC Research Programme
22	Free Vibration Analysis of Fluid Conveying Single-Walled Carbon Nanotubes	Applied Physics Letters	Vol.90, Art. 133122, April 2007	Reddy C.D.	Lu C., Rajendran S. and Liew K.M.	Large-Scale Complex Systems
23	Dynamic analysis of axially prestressed micro/nanobeam structures based on nonlocal beam theory	Journal of Applied Physics	Vol.101 (7), pages 73504-73504, April 2007	Lu P.	---	Large-Scale Complex Systems
24	Snoring source identification and snoring noise prediction	Journal of Biomechanics	Vol. 40(4), pages 861-870, April 2007	Liu Z.S.	Lou X.Y., Lee H.P. and Lu C.	Large-Scale Complex Systems
25	Further Studies on Edge Waves in Anisotropic Elastic Plates	International Journal of Solids and Structures	Vol. 44 (7-8), pages 2192-2208, April 2007	Lu P.	Chen H.B., Lee H.P. and Lu C.	Large-Scale Complex Systems
26	An Approach for the Estimation of Contact Force on a Human Head Induced by a Foreign-Object Impact	IEEE Transactions on Biomedical Engineering	Vol. 54 (1), pages 956, May, 2007	Gong S.W.	Lee H.P. and Lu C.	Large-Scale Complex Systems
27	Finite element analysis of interface delamination and buckling in thin film systems by wedge indentation	Engineering Fracture Mechanics	Vol. 74(7), pages 1118-1125, May 2007	Liu P.	Zhang Y.W., Zeng, K.Y., Lu C. and Lam K. Y.	Large-Scale Complex Systems
28	Oscillations In Intracellular Signaling Cascades	Physical Review E	Vol. 75, pages 061901, 2007	Chiam K.H.	Rajagopal G.	Large-Scale Complex Systems
29	Frequency response of a quartz crystal microbalance loaded by liquid drops	Langmuir	Vol 23, pages 7392- 7397, June 2007	Zhuang H.	Lu P., Lim S.P. and Lee H.P.	Large-Scale Complex Systems
30	Simulations Of The Spreading Of A Vesicle On A Substrate Surface Mediated By Receptor-Ligand Binding	Journal of the Mechanics and Physics of Solids	Vol. 55, pages 1166, June 2007	Liu P.	Zhang Y.W. Cheng Q.H. and Lu C.	Large-Scale Complex Systems
31	Plasma Spray Deposition on Inclined Substrates: Simulations and Experiments	Journal of Thermal Spray Technology	Vol. 16 (2), pages 261-274, June 2007	Kang C.W.	Ng H.W. and Yu S.C.M	Large-Scale Complex Systems
32	A nodal integration technique for meshfree radial point interpolation method (NIRPIM)	International Journal of Solids and Structures	Vol 44 (11-12), pages 3840-3860 Jun 1, 2007	Liu G.R.	Zhang G.Y., Wang Y.Y., Zhong Z.H., Li G.Y. and Han X.	Large-Scale Complex Systems
33	Characteristics of twodimensional flow around a rotating circular cylinder near a plane wall	Physics of Fluids	Vol 19, page 06360, Jul 2007	Cheng M.	Luo L.S.	Large-Scale Complex Systems
34	Application of Nonlocal Beam Models for Carbon Nanotubes	International Journal Of Solids And Structures	Vol 44, pages 5289-5300 Jul 2007	Lu P.	Zhang P.Q., Lee H.P. and Lu C.	Large-Scale Complex Systems
35	Molecular Dynamics Study on the Nanoimprint of Copper	Journal of Physics D: Applied Physics	Vol.40, pages 4928- 4935 Aug 2007	Pei Q.X.	Lu C. and Liu Z.S.	Large-Scale Complex Systems
36	Enhanced kidney stone fragmentation by short delay tandem conventional and modified lithotripter shock waves: a numerical analysis	Journal of Urology	Vol 178 (1), pages 314-319 Jul 2007	Tham L.M.	Lee H.P. and Lu C.	Large-Scale Complex Systems
37	Effects of Head Size and Morphology on Dynamic Responses to Impact Loading	Medical & Biological Engineering & Computing	Vol 45 (8), pages 747-757, Aug 2007	Wang F.	Lee H.P. and Lu C.	Large-Scale Complex Systems
38	A new scenario in probe local oxidation: transient pressure wave-assisted ionic spreading and oxide pattern formation	Advanced Materials	Vol 19, Issue 18 , Pages 2618 - 2623, 2007	Xie X.N.	Hong J.C., Liu Z.J., Yang S.W., Chong S.H. and Wee A.T.S	Large-Scale Complex Systems
39	Heteroepitaxial growth of quantum wire arrays through pre patterning substrate surfaces	Applied Physics Letters	Vol 91(9), page 093129, Aug 27 2007	Liu P.	Lu C., Zhang Y.W. and Lam K.Y.	Large-Scale Complex Systems
40	Formation of surface structures during heteroepitaxial thin film growth on prepatterned substrates	Physical Review B	Vol 76(8), page 085336, Aug 2007	Liu P.	Lu C. and Zhang Y.W.	Large-Scale Complex Systems
41	Numerical simulation of microdroplet formation in coflowing immiscible liquids	AICHE Journal	Vol 53 (10), pages 2534-2548, Oct 2007	Hua J.S.	Zhang B.L. and Lou J.	Large-Scale Complex Systems
42	Experimental and Computational Analysis of Droplet Formation in A High-Performance Flow-Focusing Geometry	Sensors & Actuators: APhysical	Vol 138, Issue 1, Pages 203-212, 20 July 2007	Ong W.L.	Hua J.S., Zhang B.L. and L Yobas	Large-Scale Complex Systems
43	Interaction of a Shockwave with A Non-Equilibrium Bubble: Comparison of Bem Simulations with Experiments	Journal of Fluid Mechanics	Vol 593, Pages 33-56, 2007	Klaseboer E.	Fong S.W., Turangan C.K., Khoo B.C., Sankin G.N., Szeri A.J., Calvisi M. and Zhong P.	Large-Scale Complex Systems