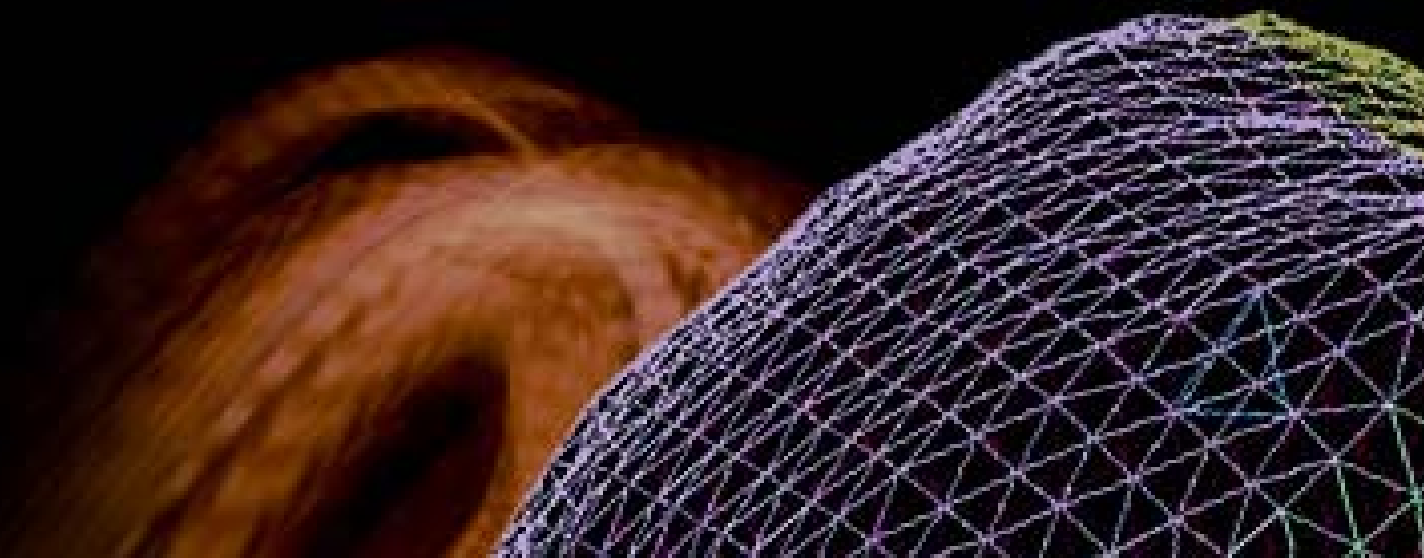


# MULTIPHYSICS 2006

14 - 15 December 2006  
Maribor, Slovenia





**MULTIPHYSICS 2006**  
**14-15 December 2006**  
**Maribor, Slovenia**

**Conference Board**

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Tehrani A, Serco Assurance, UK  
Wakes S, University of Otago, New Zealand  
Zeguer T, Jaguar, UK

## **General Information**

### **Scope of Conference**

Multiphysics analysis has been developed over the recent past to better represent the behaviour of complex processes by the use of simultaneous modelling of a number of systems. This development is driven by the industrial need to further the understanding of real physical phenomena in order to develop and design safer and more efficient products which are environmentally friendly. Such analyses and investigations were impossible to perform a number of years ago due to a lack of powerful computing systems. However, the advances in computer hardware have led to more sophisticated investigations brought about by increased computation speeds. Since this has been accompanied by new software packages which exploit the improved architecture of new generation microprocessors, there have been dramatic improvements in coupling of many mathematical simulation techniques. The objective of this conference is to discuss the findings and to explore the future trends of basic research and development as well as engineering applications in multiphysics.

The scope of the conference is to address the latest advances in theoretical developments, numerical modelling and industrial application which will promote the concept of simultaneous engineering. Typical combinations would involve a selection from subject disciplines such as Acoustics, Electrics, Explosives, Fire, Fluids, Magnetic, Soil, Structures and Thermodynamics.

### **Registration Pack – Collection Hours**

Registration packs should be collected from the Registration Desk. Collection Hours are as follows:

Wednesday, 13 <sup>th</sup> December	17:00-18:00
Thursday, 14 <sup>th</sup> December	08:00-17:00
Friday, 15 <sup>th</sup> December	08:00-17:00

### Special Events

- Wednesday 19:00  
*Welcome Reception*
- Thursday 19:00  
*Conference Banquette*

### Timing of Presentations

Each paper will be allocated 15 minutes. A good guide is 10 minutes for presentation with 5 minutes left for questions at the end.

Good timekeeping is essential, speakers are asked to keep strictly to 15 minutes per presentation.

### Language

The official language of the conference is English.

### Audiovisual

The lecture room will be preset with the following:

One laptop, one LCD projection and cables, one screen, and one microphone.

Delegates are requested to bring presentations on CD or memory stick.

### Paper Publication

Selected papers are reviewed and published in 'The International Journal of Multiphysics'.

## **Keynote Speaker**

Professor Mark Cross

### **BIOGRAPHY**

Born in London, Mark Cross graduated with a BSc (Hons) in Mathematics in 1969 followed by a PhD in Mathematical Modelling of Laser Physics Phenomena in 1972. After a short period at South Bank University in London as a Mathematics lecturer, he joined British Steel's R&D organisation to lead the development of a mathematical modelling group. His time here was formative in that he was involved in the computational modelling of a range of complex processes, the development of a range of numerical techniques and also numerical software. He then moved as a Reader to Sunderland University for 3 years and after a year in the US as a visiting professor at the Universities of Minnesota and California Berkeley, and a further year at the CFD software company CHAM, he joined the University of Greenwich.

Prof Cross was at Greenwich for over 20 years, initially as Professor of Computational Modelling, Head of the School of Mathematics, Statistics and Computing, then University Director of Research and ultimately as Pro Vice Chancellor. Whilst at Greenwich he initiated the Centre for Numerical Modelling and Process Analysis which now houses a large research programme on computational modelling and simulation. From the mid-1980s onwards his research interests increasingly involved what came to be known as *multi-physics* modelling. This involved the development of numerical methods and software technologies to facilitate coherent interaction amongst distinct phenomena, and strategies and tools to enable scalable simulation performance on parallel cluster performance computing systems. He has led the development of the PHYSICA software, now a commercial multi-physics simulation technology, and since the mid-1980s has been the Editor of the archival journal *Applied Mathematical Modelling*, published by Elsevier. The co-author of over 350 publications and the supervisor of 40+ PhD candidates, he is now the Professor of Computational Modelling in the School of Engineering at the University of Wales Swansea.

## MULTIPHYSICS 2006

Programme

<b>Time</b>	<b>Wednesday 13 Dec 06</b>	<b>Thursday 14 Dec 06</b>	<b>Friday 15 Dec 06</b>
<b>08:00</b>		<b>Registration</b>	<b>Registration</b>
<b>09:00</b>		<b>Keynote Address</b>	<b><i>Electrophysics</i></b>
<b>09:45 – 10:30</b>		<b><i>Acoustics</i></b>	
<b>10:30 – 11:00</b>		<b>Coffee Break</b>	
<b>11:00 – 12:30</b>		<b><i>Modelling Advances</i></b>	<b><i>Magnetics</i></b>
<b>12:30 – 13:30</b>		<b>Lunch</b>	
<b>13:30 – 15:00</b>		<b><i>Heat Transfer and Thermodynamics</i></b>	<b><i>Micromechanics</i></b>
<b>15:00 – 15:30</b>		<b>Tea Break</b>	
<b>15:30 – 17:00</b>		<b><i>Fluids Systems and Flow Simulation</i></b>	<b><i>Impact and Explosions</i></b>
<b>17:00</b>	<b>Registration</b>		<b>Close of Conference</b>
<b>19:00</b>	<b>Welcome Reception</b>	<b>Conference Banquette</b>	

## **Full Programme**

### **Wednesday 13 December 2006**

**17:00 Registration**

**19:00 Welcome Reception**

### **Thursday 14 December 2006**

**08:00 Registration**

**09:00 Keynote Address – Prof M Cross, University of Wales, UK**

#### **MULTI-PHYSICS MODELLING AND SIMULATION: CHALLENGES AND OPPORTUNITIES**

M Cross, T N Croft, D McBride, A K Slone and A J Williams  
*Civil and Computational Engineering Centre, School of Engineering,  
University of Wales. Swansea, UK*

**Thursday 14 December 2006**

**09:45-10:30 Acoustics**

*Chair: M. Moatamedi, University of Salford, UK*

Aero-acoustics in a tangential blower: validation of the CFD flow distribution using advanced PIV techniques

*Jean-Yves Noël – Electrolux Major Appliances Europe, Italy*

*Mark Farall – CD-adapco, Italy*

*Luca Casarsa – Università degli Studi di Udine, Italy*

Design and study of an optical fiber digital receiver

*S A Hayat, R Raza – COMSATS Institute of Information Technology, Pakistan*

*M Ajmal, Government College of Science, Pakistan*

Solving a Coupled Field Problem by Eigenmode Expansion and Finite Element Method

*Bernd Baumann, Marcus Wolff, Bernd Kost – Hamburg University of Applied Sciences, Germany*

*Hinrich Groninga - PAS-Tech GmbH, Germany*

**10:30-11:00 Coffee Break**

**Thursday 14 December 2006**

**11:00-12:30 Modelling Advances**

*Chair: M. Cross, University of Wales, UK*

LS-DYNA®: a multiphysics code

Nicolas Aquelet, Facundo Del Pin, Pierre l'Eplattenier, Art Shapiro  
*Livermore Software Technology Corp., Livermore, California, USA*

An exact percolation point of the surface-filling in even-dimensional  
Hyper-Cubic Lattices

Sasuke Miyazima – *Chubu University, Japan*

Advances in modelling congested vapour cloud explosions

Simon Chynoweth, Jonathan Puttock – *Shell Global Solutions, UK*  
Rolf Hansen, Bjorn Hjertager, Tron Solberg – *Aalborg University,  
Esbjerg, Denmark*  
Henry Weller – *OpenCFD Ltd, UK*

Underwater shock wave treatment for apples

Asuka Oda, Shigeru Itoh – *Kumamoto University, Japan*

Evaluation of SIFs for 3D interfacial crack with a wavy crack front

Andrea Piccolroaz – *Strutturale Universita' di Trento, Italy*  
Gennady Mishuris – *Rzeszow University of Technology, Poland*  
Alexander Movchan – *University of Liverpool, UK*

**12:30-13:30 Lunch**

**Thursday 14 December 2006**

**13:30-15:00 Heat Transfer and Thermodynamics**

*Chair: D. Vizman, West University of Timisoara, Romania*

Hybrid spacecraft attitude control systems

*Renuganth Varatharajoo – University Putra, Malaysia*

A fields-coupled simulation for thermal plasma flows

*Jong-Chul Lee – Wonju National College, Wonju, Korea*

*Jong-Sik Heo – Machinery and Petrochemical Research Institute,  
Sungnam, Korea*

*Youn J Kim – Sungkyunkwan University, Suwon, Korea*

Thermal dissipation of DIMM modules in Tower-BTX configuration

*Giuliano Cammarata, Giuseppe Petrone, Gaetano Sorge  
University of Catania, Italy*

Combined heat and mass transfer for drying ceramic body

*Zawati Harun, D T Gethin, R W Lewis – University of Wales,  
Swansea*

*W J Ferguson – Heriot-Watt University, Edinburgh, UK*

Finite element analysis of the temperature dependent overall conductivity  
of metallic hollow sphere structures

*Thomas Fiedler, Andreas Öchsner and Jose Grácio – University of  
Aveiro, Portugal*

**15:00-15:30 Tea Break**

**Thursday 14 December 2006**

**15:30-17:00 Fluid Systems and Flow Simulation**

*Chair: J. Noël, Electrolux Major Appliances Europe, Italy*

Regimes of direct contact condensation of steam injected into water

*A de With, R K Calay, A E Holdo, G de With*

*Fluid Mechanics Research Group, University of Hertfordshire, UK*

Simulation of particle laden flow behind a backward facing step

*Jure Ravnik, Lepold Škerget, Matjaž Hriberšek*

*University of Maribor, Slovenia*

Fluid filler influence on the behaviour of open-cell cellular structures

*Matej Vesenjajk, Zoran Ren – University of Maribor, Slovenia*

*Andreas Öchsner – University of Aveiro, Portugal*

Numerical investigation of a confined jet flow in a rectangular cavity

*Nikola Jelic – University of Innsbruck, Austria*

*Tomaž Kolšek, Jože Duhovnik – University of Ljubljana, Slovenia*

Controlled Fluid power supply system as an multiphysics system

*Darko Lovrec, Mitja Kastrevc – University of Maribor, Slovenia*

**19:00 Conference Banquette**

## **Friday 15 December 2006**

### **09:00-10:30 Electrophysics**

*Chair: N. Aquelet, Livermore Software Technology Corp., USA*

#### A three dimensional (3D) model based simulation of thermoelectric generators

Min Chen, Lasse Rosendahl, Inger Bach, Thomas Condra and John Pedersen

*Aalborg University, Denmark*

#### Interaction of shock wave produced by underwater discharge of pulsed high-current on the structure

Masahiko Otsuka, Naoki Okamoto, Shigeru Itoh – *Kumamoto University, Japan*

Hirofumi Iyama – *Yatsushiro National College of Technology, Kumamoto, Japan*

#### Simulations of secondary electron emission at tokamak divertor target plates with SOLPS-B2.5 code

Mladen Stanojevič, Jože Duhovnik – *University of Ljubljana, Slovenia*

#### Temperature dependence of electrophysical characteristics of ZnO based varistors

H Bidadli – *Islamic Azad University of Tabriz, Iran*

Sh.Hasanli – *Azerbaijan National Academy of Sciences, Baku, Azerbaijan*

H Hekmatshoar – *Sahand University of Technology, Tabriz, Iran*

#### Comparison of black-box based methods for multiphysics simulation of MEMS

Jian Guo – *University of Leeds, UK*

### **10:30-11:00 Coffee Break**

**Friday 15 December 2006**

**11:00-12:30 Magnetics**

*Chair: T. Rahulan, University of Salford, UK*

An efficient integral method for capacitance extraction of multiconductor microstrip lines

Amel Boudriga Tounsi, Khaled Grayaa and Taoufik Aguil  
*Ecole Nationale d'Ingénieurs de Tunis, Tunisia*

A study on the behaviour of underwater shock wave generated in the water container and its application to magnetic refrigeration material

Kim Young Kook, Shigeru Itoh – *Kumamoto University, Japan*

A method for simulating single charged particle motion in external magnetic and electric fields

David Eržen, Jože Duhovnik – *University of Ljubljana, Slovenia*  
John P Verboncoeur – *University of California, USA*  
Nikola Jelic – *University of Innsbruck, Austria*

Theory, applications and modelling of magnetic beads behaviour

Damasius N Fuh, Joseph I Achangwa, Walters S Niba, Waleters S  
Niba, Felicia Njweng  
*University of BUEA, Cameroon*

A comparison of magnetostatic field calculations associated with thick solenoids in the presence of iron using a Maclaurin series expansion and the complete elliptic integrals of the 1st and 2nd kind

Vasos Pavlika – *University of Westminster, UK*

**12:30-13:30 Lunch**

**Friday 15 December 2006**

**13:30-15:00 Micromechanics**

*Chair: A. Öchsner, University of Aveiro, Portugal*

Finite element solution to the Schroedinger equation

O Certik, J Plešek, C Hoeschl, J Vackar

*Academy of Sciences of the Czech Republic, Czech Republic*

Quantum-mechanical and continuum modelling of multiwall carbon nanotubes

Antonio DiCarlo, Michele Monteferrante, Luciano Teresi – *Università degli Studi 'Roma Tre', Italy*

Paolo Podio-Guidugli – *Università di Roma TorVergata, Italy*

Complex network modelling of soil pore architecture

Marko Samec, Dean Korošak – *University of Maribor, Slovenia*

Sacha Jon Mooney – *University of Nottingham, UK*

Radiating effect of participating media in a flameless industrial reactor

Giuliano Cammarata, Giuseppe Petrone, Luca Romano – *University of Catania, Italy*

3D modeling of thermal convection in industrial Czochralski-like configurations

Daniel Vizman – *West University of Timisoara, Romania*

**15:00-15:30 Tea Break**

**Friday 15 December 2006**

**15:30-17:00 Impact and Explosions**

*Chair: Z. Ren, University of Maribor, Slovenia*

Impact biomechanics of the abdominal cavity and abdominal injury criteria

Iztok Ciglarič, Sanid Emšo, Hermann Steffan – *Graz University of Technology, Austria*

Composite structures subjected to transient dynamic loading

P R Hampson, M Moatamedi – *University of Salford, Manchester, UK*

On mechanism of non-heating sterilization using the underwater shock wave loading and gas-formation

A Takemoto, M Otsuka, S Itoh – *Kumamoto University, Japan*  
Y Mibuka, M Iwahara – *Sojo University, Japan*

Verification of numerical dispersion analysis by a two cylinders impact problem

Dusan Gabriel, Jiri Plesek, Radek Kolman, Miloslav Okrouhlik, Frantisek Vales – *Academy of Sciences, Praha, Czech Republic*  
Matjaž Šraml – *University of Maribor, Slovenia*

Numerical Simulation of a metal sheet during explosive forming

Hideki Hamashima, Takeshi Hinata, Hirofumi Hamada, Shigeru Itoh  
*Kumamoto University, Japan*

**17:00 Close of Conference**

# **Keynote Address**

THURSDAY 14 DECEMBER 2006  
09:00 - 09:45

CHAIR:

Dr. M. Moatamedi  
University of Salford  
UK

Thursday, 14 December 2006

09:00 – 09:45

## **Keynote Address**

### **MULTI-PHYSICS MODELLING AND SIMULATION: CHALLENGES AND OPPORTUNITIES**

M Cross, T N Croft, D McBride, A K Slone and A J Williams  
*Civil and Computational Engineering Centre, School of Engineering,  
University of Wales. Swansea, UK*

During the last decade there has been a substantial development in the computational modelling of engineering processes that involve the interaction amongst a range of phenomena. Such problems might involve the interaction amongst any of fluids, structures, thermal, acoustic and electromagnetic fields. Although the computational modelling community is well experienced in the modelling of single phenomena and even thermo-fluids and thermo-structural interactions, other coupled phenomena are less straightforward. These are very challenging problems especially since differing groups of interacting physics may well be operating at distinctive time and length scales. Hence, addressing such problems requires far more than simply 'hooking' the output from one phenomena specific code as input into another. Furthermore, the compute challenges of multi-physics are very significant in terms of both computational effort and the large data sets that are generated and then need mining with visualisation technology.

This contribution addresses the above issues and describes one attempt at the development of multi-physics simulation technologies, together with some successes and failures, especially across multiple time and length scales. It also addresses what has to be achieved if closely coupled multi-physics simulation is to be realised that captures the actual physics in a time and space accurate fashion.

# **Acoustics**

THURSDAY 14 DECEMBER 2006  
09:45 - 10:30

CHAIR:

Dr. M. Moatamedi  
University of Salford  
UK

## **Aero-acoustics in a tangential blower: validation of the CFD flow distribution using advanced PIV techniques**

Jean-Yves Noël (1), Mark Farall (2), Luca Casarsa (3)

*(1) Electrolus Major Appliances Europe, (2) CD-adapco, (3) Dipartimento di Energetica e Macchine, Università degli Studi di Udine, Italy*

Noise reduction is of increasing importance to customers. As such, the development of aero-acoustics is gaining special focus within industry. Computational Aero-Acoustics (CAA), the coupling of Computational Fluid Dynamics (CFD) and Computational Acoustics (CA), is being used in the design and assessment of a range of products from HVAC ducts to domestic appliances.

The process for carrying out an Aero-Acoustic simulation begins with the solution of the transient flow dynamics in order to compute accurately the pressure fluctuations at a number of points in the computational domain. These fluctuations are passed to the acoustic code to propagate the acoustic waves through the system and determine its acoustic signature. To minimize errors in the acoustic propagation analysis it is thus essential that accurate predictions of the noise sources be obtained.

This paper concentrates on the CFD part of the aero-acoustic simulation. The case considered has been taken from the European project DESTINY:3 and comprises a tangential blower located inside a complex duct system. Air is drawn into the fan through two inlets and exits through a single duct. The computational methodology and flow field predictions are presented and compared to experimental PIV data. The numerical predictions were found to be in good agreement with the experimental data, reproducing the asymmetries in the flow field.

## **Design and study of an optical fiber digital receiver**

S A Hayat (1), M Ajmal (2), R Raza (1)

*(1) COMSATS Institute of Information Technology, Pakistan, (2) Government College of Science, Pakistan*

An optical fiber digital receiver was designed for audible frequency range. There were some parameters measured like bandwidth, intensity and attenuation. We have been succeeded to achieve various educational and practical purposes, which were regarding to this project. The experiment helps us to aware optical detector, optical fiber and frequency to voltage converter

Key words: Optical Fiber, Analog communication, Digital communication, optical detector

## **Solving a Coupled Field Problem by Eigenmode Expansion and Finite Element Method**

Bernd Baumann (1), Marcus Wolff (1,2), Bernd Kost (1), Hinrich Groninga (2)  
*(1) Hamburg University of Applied Sciences, Faculty of Engineering & Computer (2) PAS-Tech GmbH*

The propagation of sound in fluids is governed by a set of coupled partial differential equations supplemented by an appropriate equation of state. In many cases of practical importance one restricts attention to the case of ideal fluids with vanishing transport coefficients. Then the differential equations decouple and sound propagation can be described by the wave equation. However, when loss mechanisms are important, this is in general not possible and the full set of equations has to be considered.

For photoacoustic cells an alternative procedure has been used for the calculation of the photoacoustic signal of cylinder shaped cells. The method is based on an expansion of the sound pressure in terms of eigenmodes and the incorporation of loss through quality factors of various physical origins. In this paper we demonstrate, that the method can successfully be applied to the finite element calculation of the signal of photoacoustic cells of unconventional geometry.

# **Modelling Advances**

THURSDAY 14 DECEMBER 2006  
11:00 - 12:30

CHAIR:

M. Cross  
University of Wales  
UK

## **LS-DYNA®: a multiphysics code**

Nicolas Aquelet, Facundo Del Pin, Pierre l'Eplattenier, Art Shapiro  
*Livermore Software Technology Corp., Livermore, California, USA*

Several modules are being separately developed or are currently implemented in LS\_DYNA® to treat complex multiphysics simulations:

- A new Fluid Mechanics approach will be introduced in future versions of LS-DYNA® to solve incompressible flows. The objective of this new formulation will be to solve fluid-structure interaction problems using Lagrangian interfaces. Since the mesh follows the material, for large deformations a very robust and fast re-meshing tool is being created.
- An alternative solution is solving the material large deformations with a multi-material ALE formulation, for which the mesh motion is independent of the material dynamics. This method available in LS-DYNA® is coupled with an updated Lagrangian finite element formulation to model fast dynamic fluid-structure problems. The fluid-structure coupling method, namely Euler-Lagrange coupling, allows the modeling of fluid-structure interaction problems, in which Lagrangian structures are superimposed to ALE meshes for fluids.

## **An exact percolation point of the surface-filling in even-dimensional Hyper-Cubic Lattices**

Sasuke Miyazima

*Department of Natural Science, Chubu University, Japan*

An exact percolation threshold of a hyper-cubic lattice in the even  $(2n)$  - dimensional space is obtained to be  $P_c = 0.5$ , if we distribute a unit cell of  $n$ -dimensional structure in the  $2n$ -dimensional hyper-cube instead of a particle or a bond in 2-dimensional lattice, where only exact threshold has been obtained. We can obtain an exact threshold value of percolation in the even-dimensional hyper-cubic lattice, because of the existence of self-dual lattice in  $2n$ -dimension space and the orthogonal relation of  $(2n - n)$ -dimension structures in the original and the dual hyper-cubic lattices.

As an example we consider a 4-dimensional hyper-cubic lattice, where we distribute squares in the hyper-cubic lattice with four lattice points  $(i, j, k, l)$ ,  $(i+1, j, k, l)$ ,  $(i, j+1, k, l)$ ,  $(i+1, j+1, k, l)$ . The corresponding square in the dual hyper-cubic lattice is  $(i+1/2, j+1/2, k+1/2, l+1/2)$ ,  $(i+1/2, j+1/2, k+3/2, l+1/2)$ ,  $(i+1/2, j+1/2, k+1/2, l+3/2)$ ,  $(i+1/2, j+1/2, k+3/2, l+3/2)$ , where it is important fact that once we choose a square in either lattice, we can determine a corresponding square without ambiguity

## **Advances in modelling congested vapour cloud explosions**

Simon Chynoweth (1), Rolf Hansen (2), Bjorn Hjertager (2), Jonathan Puttock (1), Tron Solberg (2) and Henry Weller (3)  
*(1) Shell Global Solutions (UK), (2) Aalborg University, Esbjerg, Denmark, (3) OpenCFD Ltd, UK*

Designing industrial plant to process flammable fluids requires understanding of the effects of an accidental release of those fluids. One potential consequence is a vapour cloud explosion in which the turbulence, and hence the severity, is greatly enhanced by the presence of congestion associated with steelwork, pipes and other process equipment. The severity of the explosion is also affected by the way in which fluid disperses from the release. The impact on people can depend on the propagation of the blast wave and its interaction with the structure of nearby occupied buildings.

The three-dimensional simulation of such events is hindered by the range of interacting physical processes and scales of motion. The state of the art in modelling these processes is to use Computational Fluid Dynamics for the larger (resolvable) scales together with parameterisation of the small, unresolvable scales.

Recently, OpenFOAM, an open-source library of tools for solving mathematical descriptions of physical problems, has become available. This paper discusses initial results from the application of OpenFOAM to explosion modelling and the ways in which this approach might offer a step change in our ability to simulate such processes.

## **Underwater shock wave treatment for apples**

Asuka Oda (1), Shigeru Itoh (2)

*(1) Graduate School of Sciences and Technology, Kumamoto University, Japan, (2) Shock Wave and Condensed Matter Research Center, Kumamoto University, Japan*

Underwater shock wave is easily generated by means of explosion of explosives or high voltage electric discharge under water. Underwater shock wave can break inside of material without outside damage of that, because it has properties of high pressure, very short duration of action, and passing through a material. The purpose of this study is improvement of foods using properties of underwater shock wave. We study about improvement of foods using underwater shock wave. A detonating fuse and an electric detonator were used for generation of underwater shock wave, and apples were used as one of food sample. Moreover the behavior of underwater shock wave for an apple was investigated by optical observation. The following results were obtained: extraction of juice was improved, because apples softened. And amount of phenolics components in juice of treatment samples was increased in comparison with that of control samples. It is considered that the result of underwater shock wave treatment for apples is new possibility in food processing due to underwater shock wave.

## **Evaluation of SIFs for 3D interfacial crack with a wavy crack front**

Andrea Piccolroaz (1), Gennady Mishuris (2), Alexander Movchan (3)

*(1) Dipartimento di Ingegneria Meccanica e Strutturale Universita' di Trento, Italy, (2) Department of Mathematics, Rzeszow University of Technology, Poland, (3) Division of Applied Mathematics, Department of Mathematical Sciences, Liverpool, UK*

The problem of a semi-infinite plane crack along the interface between two 3D isotropic half-spaces is considered here. The two characteristic features of this problem are the coupling of all three opening modes and the oscillatory behaviour of the solution near the crack edge. For this problem two issues are of major interest: the representation of the stress intensity factors, and the expression of the variation of stress intensity factors arising from an infinitesimal coplanar perturbation of the crack front. Two methods of solution have been considered in the past: Lazarus and Leblond (1998) applied the "special" method by Bueckner and found the expression of the variation of the stress intensity factors without solving the complete elasticity problem; their final formulas are simple and elegant, expressed in terms of the physical variables, but have the disadvantage of involving five unknown constants; on the other hand the "general" solution to the problem has been recently addressed by Bercial-Velez et al. (2005).

We reformulate the weight functions introduced by Bercial-Velez et al. (2005) with the right order of homogeneity. Then, using a new representation of the Betti identity introduced by Willis and Movchan (1995), we obtain explicit formulas for the evaluation of the SIFs and also for the constants in the second term asymptotics of stress and displacement fields.

Finally, we derive the variation of SIFs for a wavy crack, which puts us in a position to find the exact representation of the constants appearing in Lazarus-Leblond's formulation.

Key words: stress intensity factors; interfacial crack; crack front perturbation

# **Heat Transfer and** **Thermodynamics**

THURSDAY 14 DECEMBER 2006  
13:30 - 15:00

CHAIR:

D. Vizman  
West University of Timisoara  
Romania

## Hybrid spacecraft attitude control systems

Renuganth Varatharajoo

*Department of Aerospace Engineering, University Putra Malaysia*

The spacecraft missions are becoming more challenging in the recent years. Additionally, the requirements for space missions in terms of their performances are also gradually increasing. Therefore, the spacecraft have received attention for further optimisation. An approach would be to enhance the capabilities of each existing sub-system without altering the overall mass and volume budgets as in the same level today. Recent technology advances have triggered an appreciable enthusiasm towards off-the-shelf spacecraft subsystem concepts. The idea of combining the conventional Attitude Control System and the Electrical Power System is presented in this article. The Combined Energy and Attitude Control System (CEACS) consisting of a double counter rotating flywheel assembly is investigated for small satellites in this article. Another hybrid system incorporating the conventional Attitude Control System into the Thermal Control System forming the Combined Attitude and Thermal Control System (CATCS) is also investigated for small satellites herein. The CATCS consists of an electric conducting fluid that circulates in a closed loop (fluid wheel) simultaneously serving for the attitude and thermal controls. The governing equations describing both these novel hybrid subsystems are presented and their onboard architectures are numerically tested for their attitude performances. Both the investigated novel hybrid spacecraft subsystems comply with the reference mission requirements. Hence, the commissioning of these hybrid subsystems on the future spacecraft would benefit the missions, e.g., life duration, reliability and performance enhancements, mass and volume savings, etc.

Key words: Attitude Control/Energy Storage/Thermal Control/Flywheel/Fluid Wheel

## **A fields-coupled simulation for thermal plasma flows**

Jong-Chul Lee (1), Jong-Sik Heo (2), and Youn J Kim (3)

*(1) Department of Automotive Engineering, Wonju National College, Wonju, Korea (2) Machinery and Petrochemical Research Institute, Sunghnam, Korea, (3) School of Mechanical Engineering, Sungkyunkwan University, Suwon, Korea*

The electrodes erosion is indispensable for atmospheric plasma systems as well as switching phenomena of arc plasmas due to heat flux entraining from the high temperature zone. But the experimental and theoretical works are not easy to realize the characteristic phenomena due to the complex physical processes included with. In this study, we analyzed the electrical conductivity and the temperature of arc plasmas between the electrodes using the computational techniques, which are coupled with the thermal-flow and electromagnetic fields. Numerical results show that the behavior of arc plasmas is very sensitive to the existence of electrode vapors, and it also affects the capability of plasma systems critically.

Key words: Atmospheric thermal plasma, CFD, Ohmic heating, electrode erosion, metallic vapor

## **Thermal dissipation of DIMM modules in Tower-BTX configuration**

Giuliano cammarata, Giuseppe Petrone, Gaetano Sorge  
*Department of Industrial and mechanical Engineering, University of Catania, Italy*

Natural convection for Dual In-Line Memory Module (DIMM) systems, disposed as predicted by the recent Balanced Technology Extended (BTX) form factor in tower configuration, is numerically studied in this communication. These physical systems can be represented by horizontal air-filled layers bounded by parallel walls in which multiple heat sources are present. In order to investigate on the thermal performances of the considered electronic equipments, several 2D and 3D steady and time-dependent numerical models are proposed. Numerical models are developed by using a FEM multiphysical commercial software while computations are carried-out on a 64 bit calculator of 16 GB of RAM. The results, obtained for different ambient temperature values and imposed operative conditions (power supplied to the memories), show as thermo-convective instabilities may be produced and consequently different kinds of fluid motion field could be detected. Heat transfer parameters are studied as function of the number of the DIMM considered in the numerical model and the number of chips for each DIMM. A sixth order polynomial fitting law is for the first time proposed in order to correlate, for the analysed physical systems, the maximum temperature produced on the chips and the supplied power to the electronic device. This study could be an useful tool for investigation on critical cooling conditions for BTX form factor computers or for innovative projects of fan-less computers architecture.

Key words: Electronic equipment cooling, thermo-convective instabilities

## **Combined heat and mass transfer for drying ceramic body**

Zawati Harun (1), D T Gethin (1), R W Lewis (1), W J Ferguson (2)

*(1) Civil and Computational Engineering Centre, University of Wales, Singleton park, Swansea, UK, (2) School of the Built Environment, Heriot-Watt University, Edinburgh, UK*

In this work, a two-dimensional numerical model of heat and mass transfer for the convective drying process of ceramic material was developed. The governing system of fully coupled non-linear partial differential equations describing the process was derived from a mechanistic approach along with the influence microscopic effect (temperature gradient in the pore) during the vapour transfer. The most extensive formulation of moisture transport variables used in many hygro-thermal and soil transport investigations was adopted as the basis for further development in this work. Through the verification and validation of the results calculation, showed that the measured variables and coefficients (diffusivity) in heat and mass transport properties strongly depend on the right input of heat and mass transport variables formulation or derivation either in macroscopic or microscopic scale.

Key words: convective drying, coupled heat and mass transfer, transport variables, microscopic effect

## **Finite element analysis of the temperature dependent overall conductivity of metallic hollow sphere structures**

T Fiedler, A Öchsner and Grácio

*Department of Mechanical Engineering, centre for Mechanical Technology and Automation, University of Aveiro, Portugal*

In the scope of this study, finite element analysis is applied in order to determine the effective thermal conductivity of periodic metallic hollow sphere structures (MHSS). Hollow sphere structures constitute an innovative group of advanced composite materials. Their characteristics comprise high specific stiffness, good damping properties, energy absorption and thermal insulation. Combination of these properties opens a wide field of potential multifunctional applications e.g. in automotive or aerospace industry. Hollow sphere structures are assembled by single metallic hollow spheres. The coherence of the hollow spheres can be achieved by different joining technologies such as sintering and adhesion. Consequently, the thermal characteristics of the structure depend on the geometry of the structure and thermal properties of the base materials. The high closed porosity of the structure in combination with a low thermal conductivity of an epoxy resin suggests the application of such materials for thermal insulation. For the determination of the thermal conductivity of the MHSS, the temperature dependence of the thermal conductivities of the base materials, i.e. hollow spheres and joining element, are considered. Two different cases, a low and a high temperature gradient within the structure are distinguished. Furthermore, the overall thermal conductivities of sandwich panels with an insulating MHSS core in dependence on the relative face sheet thickness are investigated.

# **Fluid Systems and Flow** **Simulation**

THURSDAY 14 DECEMBER 2006  
15:30 - 17:00

CHAIR:

J. Noël  
Electrolux Major Appliances Europe  
Italy

## **Regimes of direct contact condensation of steam injected into water**

A de With, R K Calay, A E Holdo, G de With  
*Fluid Mechanics Research Group, University of Hertfordshire, UK*

Direct contact condensation of steam injected into water is a special mode of condensation where condensation occurs on the interface between steam and water. This type of condensation forms an essential part of various industrial applications and correct modelling of the condensation is necessary to obtain an optimised design of these devices.

Crucial in the modelling of direct contact condensation is the behaviour of the injected steam, commonly termed as a regime. Depending on the environmental conditions, steam injected into water appears in different regimes. These are observed in different geometrical appearances of the injected steam and are ranging from steam being condensed in the injector to bubbles and jets of steam formed in water.

The two dimensional regime maps and models presently available are able to predict different condensation behaviour for limited flow conditions.

In this paper the new three-dimensional condensation regime diagram is presented, capable of predicting regimes at different flow conditions of steam and water and for different sizes of steam injector. Furthermore, expected penetration distance of steam injected into water, which is also crucial in modelling of the process, is presented for different flow conditions in the form of a new two-dimensional steam plume length diagram.

## **Simulation of particle laden flow behind a backward facing step**

Jure Ravnik, Lepold Skerget, Matjaz Hribersek  
*University of Maribor, Faculty of Mechanical Engineering, Maribor*

In the paper we present a numerical method for solving planar laminar flows laden with massless particles. The Navier-Stokes equations are written in a velocity-vorticity form and solved in a time dependent manner by a combination of the boundary element method, finite element method and wavelet transform. Wavelet compression is used to decrease memory requirements and accelerate the boundary element method solution of the flow kinematics equation. On the other hand, the vorticity transport equation is solved by the finite element method. A non-linear iteration loop is used to tackle the nonlinearity in the system.

Particles are considered to be massless, their positions are simulated in a Lagrangian manner using the converged flow field of each time step. As a numerical example showing the versatility of our numerical scheme, we consider a time dependent flow of an incompressible viscous fluid over a backward facing step. The flow forms a vortex street behind the step, into which the particles are inserted.

Key words: backward facing step, massless particles, boundary element backward facing step, massless particles, boundary element method

## **Fluid filler influence on the behaviour of open-cell cellular structures**

M Vesenjāk (1), A. Öchsner (2), Z Ren (1)

*(1) University of Maribor, Faculty of Mechanical Engineering, Maribor, Slovenia (2) University of Aveiro, Portugal*

Computational simulations of regular open-cell cellular structures accounting for fluid fillers are presented in this paper. The purpose of this research was to determine the influence of the fluid filler on the macroscopic behaviour of the cellular structure under uniaxial impact loading conditions. Different relative densities, sizes of cellular structures and filler viscosities at high strain rates have been considered. The fluid flow through the open-cell cellular material was modelled and analyzed with the explicit code LS-DYNA. The fluid was modelled by applying a Smoothed Particle Hydrodynamics (SPH) method using a fully coupled interaction between the base material and the fluid filler. The SPH model has been compared and evaluated with the computational fluid dynamics code ANSYS CFX. Computational results have shown that the influence of the filler increases with increase of the relative density. It was also proven that the size of the cellular structure and the number of cells significantly influence the filler flow and with that the global behaviour of the cellular structure.

## **Numerical investigation of a confined jet flow in a rectangular cavity**

Nikola Jelic (1), Tomaž Kolšek(2), Jože Duhovnik (2)

*(1) Institute for Theoretical Physics, University of Innesbruck, Austria*

*(2) Department of Computer Aided Design LECAD, Faculty of Mechanical Engineering, University of Ljubljana, Slovenia*

We present the results of investigation of a low-Reynolds number incompressible fluid flow in a rectangular two-dimensional cavity. It has been shown that the behaviour of the flow may be controlled by the cavity length and width. Depending on the ratio between the length ( $L$ ) and width ( $w$ ) of the chamber the flow is either steady or non-steady. It has been found that for small chamber lengths the flow is steady and geometrically symmetric. Increased chamber lengths lead to unsteady flows with oscillating and hardly predictable jet flow pattern. Further increase of the chamber length leads again to steady but asymmetric flow. These observations are useful for possible control of the jet behaviour under various conditions. This research is relevant for both basic jet-flow investigations as well as for industrial purposes. The sensitivity of the solution to perturbation of simulation parameters is identified as an important issue to be attacked in future by both experimental and numerical means.

Key words: confined jet, fluid flow, self sustained oscillations, CFD

## **Controlled Fluid power supply system as an multiphysics system**

Darko Lovrec, Mitja Kastrevc

*University of Maribor, Faculty of Mechanical Engineering, Slovenia*

Contemporary industrial applications of the electro-hydraulic supply systems, to be applied e.g. on the tool and metal shaping machines, requires high power transmission capacity at low losses of energy, low noise emission and convenient price-performance ratio. A principle of volumetric control of the hydraulic energy –hydraulic adjusted supply systems have proven to be suitable to satisfy above requirements.

Such systems can be in principle controlled at the hydraulic or electric side in order to control flow or consequently pressure of the medium. Constant speed induction motors in combination with an adjustable pump displacement volume is a common used application. Constant displacement volume pumps in combination with a variable rotational speed motor, on other hand, becomes increasingly used in praxis due to its attractive price.

The main purpose of the work is to present theoretical and experimental analysis of suggested application of controlled electro hydraulic supply system on metal shaping machines – with an exact mathematic model of the supply system. It is well-known that the modelling of such complex systems, including the interference of hydraulic (hydraulic fluid and mechanics components), electronics, control techniques and sensor technology, with all the reciprocate influences and interactions, is a very demanding task. The subject of different degrees of accuracy when modelling different parts of hydraulic systems has been well described by several authors, where only a simplified modelling is usually applied. These types of mathematical models can produce good results only for the basic simulation and behaviour description of the system. Therefore a detailed description of the complex system and appropriate mathematical models with all nonlinearities and specialities of the components is needed, as presented in the work.

Key words: servohydraulic, adaptive supply system, mathematical modelling, computer simulation, experiment

# **Electrophysics**

FRIDAY 15 DECEMBER 2006  
09:00 - 10:30

CHAIR:

N. Aquelet  
Livermore Software Technology Corp.  
USA

## **A three dimensional (3D) model based simulation of thermoelectric generators**

Min Chen, Lasse Rosendahl, Inger Bach, Thomas Condra and John Pedersen  
*Aalborg University, Denmark*

Inside a thermoelectric generator (TEG) the thermal field and the electric field are strongly coupled with each other. Not only is the Seebeck effect of temperature difference resulting in electric field of interest but the electric current flowing in the thermoelectric material causing heat through Joule and Peltier loss is also important. This multi-physics effect therefore must be taken into account in the modelling and simulation of a TEG in order to obtain the optimum design of it.

There are two kinds of governing equation currently used in thermoelectric numerical modelling and simulation. One is based upon irreversible thermodynamics whilst the other is derived from heat transfer theory. This paper analyses the benefits and drawbacks of the two methods, over the control elements and at boundaries, respectively. Bearing the difference in mind, we realize a 3D simulation of TEG using the heat transfer governing equation. The simulation results are compared and discussed with some previously reported results.

Key words: three dimensional, thermoelectric generators, governing equation

## **Interaction of shock wave produced by underwater discharge of pulsed high-current on the structure**

Masahiko Otsuka (1), Naoki Okamoto(1), Hirofumi Iyama (2) and Shigeru Itoh (3)

*(1) Graduate School of Sciences and Technology, Kumamoto University*

*(2) Department of Mechanical and Electrical Engineering, Yatsushiro National College of Technology, Kumamoto (3) Shock Wave and Condensed Matter Research Center, Kumamoto, Japan*

Pulsed power is a short pulse, high energy generated by an explosive charge or high current which can be utilized for various applications. However, the usage of explosives is very severe and also it is necessary to strive for the handling, maintenance and safety of explosives. Rather than using explosive, electric pulsed power can be used to generate shock waves, as the technique is simple and safe. The aim of this study is to effectively use the underwater shock wave generated by the electric pulsed power for the destruction of structure and rocks. In this study, the underwater shock wave produced by gap discharge (GD method) or metal wire explosion (WE method) is evaluated by optical observation and pressure measurement. Results of the investigation for the underwater shock wave are then compared to a numerical simulation of the same problem.

The energy of an underwater shock wave can be improved by increasing the charge energy of a capacitor. The GD method showed the existence of many shock waves. The duration of the pressure pulse is long in this phenomenon, but a peak pressure of underwater shock wave by the WE method is higher than the GD method.

Key words: Pulsed power, Plasma, Underwater shock wave

## **Simulations of secondary electron emission at tokamak divertor target plates with SOLPS-B2.5 code**

Mladen Stanojevič and Jože Duhovnik

*University of Ljubljana, Faculty of Mechanical Engineering, LECAD  
Laboratory, Ljubljana, Slovenia*

Integrated modelling and simulations of tokamak fusion reactors require taking into consideration phenomena from various fields of physics. In this paper we analyse the secondary electron emission at tokamak divertor target plates and its influence on tokamak edge plasma parameters. This is an important surface effect that may significantly influence our capability to control particle and energy fluxes between the plasma and the surrounding environment. We implemented three different optional models of the secondary electron emission in the SOLPS-B2.5 code, namely, a constant value and two semi-analytical secondary electron emission models, based on the studies of Subba et al. [Plasma Phys. Control. Fusion, 44 (2002), 61-70] and Ordonez and Peterkin, Jr. [J. Appl. Phys., 79 (1996), 2270-2274]. SOLPS-B2.5 is a two-dimensional plasma fluid transport code, in which the transport equations are solved in the poloidal plane assuming uniformity in the toroidal direction. Simulations of the tokamak boundary plasma applying each of the secondary electron emission models mentioned above and two optional divertor surface materials relevant to the envisaged ITER reactor, i.e., carbon and tungsten, were performed for the ASDEX Upgrade tokamak shot No. 16151, which is considered as a benchmark case for simulating so-called L-mode plasmas in single divertor tokamaks.

Key words: plasma, tokamak, fusion, simulation, secondary electron emission, divertor, fluid transport code

## **Temperature dependence of electrophysical characteristics of ZnO based varistors**

H Bidadi (1), Sh.Hasanli (2) and H Hekmatshoar (3)

*(1) Department of Physics, Islamic Azad University of Tabriz, Tabriz-Iran, (2) Institute of Physics, Azerbaijan National Academy of Sciences, Baku-Azerbaijan, (3) Department of Physics, Sahand University of Technology, Tabriz-Iran*

The present work is devoted to studying the effect of temperature on current-voltage characteristics and electrical conductivity of ZnO based varistors. It is shown that the observed nonlinear current-voltage characteristics (CVC), exponential dependence of electric conductivity, nonlinearity factor and also reduction of samples opening voltage are connected with the ZnO grain boundaries. The observed hysteresis loops in the current-voltage characteristics of the samples in all temperature intervals where their width is increased by increasing the temperature is explained on the basis of the existing dipole moments of added oxide impurities of the type Co and Mn.

Key words: Varistors, nonlinearity, electrical conductivity, hysteresis, ZnO

## **Comparison of black-box based methods for multiphysics simulation of MEMS**

Jian Guo

*School of Mechanical Engineering, University of Leeds, UK*

The rapid progress of Micro-Electro-Mechanical-Systems (MEMS) industry has growing demands for multiphysics simulations. In order to improve the efficiency, a desirable multiphysics simulation tool should be black-box based, i.e. be able to utilize commercially or academically available phenomena specific solvers for each physical field. Several numerical techniques have been developed so far for black-box based multiphysics simulations of MEMS devices, the key objectives of this paper are to compare these techniques, especially the recently presented Relaxation with Steffenson's Acceleration (RSA) scheme developed by the author, and to give guidance on selecting the suitable method for black-box based multiphysics simulation. In this paper, three available black-box based multiphysics simulation methods, i.e. the Relaxation, the Multilevel Newton and the Quasi-Newton, are reviewed, then the theoretic background of the RSA scheme is described in detail. For the purpose of quantitative comparisons, these approaches are used to combine FE-based structural solver with BE-based electrostatic solver for multiphysics simulations of MEMS electrostatic actuators. The results show that the latter three approaches all take much less iterations than the Relaxation method for strong coupled or nonlinear situations. However, the RSA scheme needs less computing loads within each iteration and keeps the advantage of easy programming.

Key words: Multiphysics Simulation, MEMS.

# **Magnetics**

FRIDAY 15 DECEMBER 2006  
11:00 - 12:30

CHAIR:

T. Rahulan  
University of Salford  
UK

## **An efficient integral method for capacitance extraction of multiconductor microstrip lines**

Amel Boudriga Tounsi, Khaled Grayaa and Taoufik Aguil  
*Ecole Nationale d'Ingénieurs de Tunis, Tunisia*

A new integral method is developed to analyse multiconductor microstrip lines in quasi-static. This technique is based on the generalised equivalent circuits by using transverse admittance operators. In conjunction with wavelets, this approach evaluates the accurate determination of capacitance matrix. A set of integral equations is obtained Using Galerkin's method with the unknown total charge distribution expanded in terms of compactly-supported wavelets. Thus a sparse matrix equation is developed. It is also proven that a significant reduction of computational time and memory storage are obtained. Numerical results are in good agreement with those in previous publications. This accurate technique is simple and easy to implement. It is believed to be useful in the design of high speed integrated circuits interconnects.

Key words: Integral method; quasi static; multiconductor microstrip lines; wavelets; capacitance

## **A study on the behaviour of underwater shock wave generated in the water container and its application to magnetic refrigeration material**

Kim Young Kook (1), Shigeru Itoh (2)

*(1) Graduate School of Science and Technology, Kumamoto University,*

*Japan (2) Shock Wave and Condensed Matter Research Center, Kumamoto University, Japan*

Most of composite materials are made by sintering method. In this research, in order to make composite material for magnetic refrigeration, we carried out several experiments for the powder consolidation using the shock compaction method and numerical analysis for the behavior of underwater shock wave. The shock compaction method is to consolidate metal powders using underwater shock wave including an ultra-high pressure and high velocity generated by detonation of explosive. Generally, the magnitude of peak pressure and the pressure distribution of underwater shock wave depend on water container which is one of the parts of high pressure generating device. In this study, also we have investigated several water containers using numerical analysis and observation experiment. As results, underwater shock wave is affected by the reflected wave occurred by inner angle of water container and the magnitude of reflected wave in the water container depends on the inner angle of water container. The pressure and velocity of reflected wave is gradually decreased with increasing inner angle of water container.

Key words: Shock compaction Method, Underwater shock wave, Powder consolidation

## **A method for simulating single charged particle motion in external magnetic and electric fields**

David Erzen (1), John P Verboncoeur (2), Joze Duhovnik (3), Nikola Jelic (4)  
*(1) Faculty of Mechanical Engineering, University of Ljubljana, Slovenia (2) Dept Nuclear Engineering, University of California, USA, (3) Faculty of Mechanical Engineering, University of Ljubljana, Slovenia, (4) Dept of Theoretical Physics, University of Innsbruck, Austria*

In this paper we present a new software package for computational simulation of single particle motion in the presence of static external electric and magnetic fields. This seemingly simple problem is in fact very complicated. Namely, while analytic formulations of this problem are unambiguous, it is very difficult to predict even qualitatively a charged particle trajectory for an arbitrary combination of field parameters, except in simplified cases. Instead, one might perform a single particle motion simulation. Our software package represents a unique tool for this problem. A special new feature of our approach is constructing the instant Larmor Center Trajectory. For the case of slowly changing fields, the Larmor center trajectory reduces to the less general guiding center trajectory approximation. The possibilities for further investigating these two approaches by using our software might be of great interest for both educational and engineering purposes, especially in the areas of gaseous electronics and laboratory, fusion and space plasmas.

Key words: charged particle motion, numerical simulations, guiding center, Larmor center, magnetic field, electric field, adiabatic invariants

## **Theory, applications and modelling of magnetic beads behaviour**

Damasius N Fuh, Joseph I Achangwa, Walters S Niba, Felicia Njweng  
*University of BUEA, Cameroon*

The studying and manipulating macromolecules like DNA by researchers will help in the application of microfluidics to biotechnology which include proteins and cells in vitro and within living organisms. Thereby presenting an enlightening balance of numerical approaches, theory, and experimental examples, this cutting-edge resource offers keen insight into this burgeoning field.

This abstracts sites detail on the mechanical behavior of the different types of micro/nano particles and macromolecules that are used in biotechnology. Focusing on microfluidics theory and the mechanics of microflows and microdrops giving a faster understanding to this and also a concrete studies on the transport and dispersion of biochemical species and particles helps in realising model biochemical reactions, including DNA hybridization and enzymatic reactions.

This abstract helps in mastering the theory, applications, and modeling of magnetic beads behavior and provides an overview of self-assembly and magnetic composite.

## **A Comparison of Magnetostatic Field calculations associated with thick Solenoids in the Presence of Iron using a Maclaurin Series expansion and the Complete Elliptic Integrals of the 1st and 2nd kind**

Vasos Pavlika

*Harrow School of Computer Science, University of Westminster, UK*

The effect of iron on the uniformity of the field produced by an axisymmetric thick solenoid is considered. Using a Maclaurin series expansion the solution to the vector potential is found and from this the magnetic induction  $B$  is derived. The solution to the vector potential and field components is also achieved using the complete Elliptic Integrals of Legendre of the first and second kind respectively with numerical results using both methods of solution computed.

Key words: Time independent field, Elliptic Integrals of the first and second kind, Maclaurin Series expansion

# **Micromechanics**

FRIDAY 15 DECEMBER 2006  
13:30 - 15:00

CHAIR:

A. Öchsner  
University of Aveiro  
Portugal

## Finite element solution to the Schroedinger equation

O Certik (1) , J Plesek (2), C Hoeschl (2), J Vackar (1)  
*Academy of Sciences of the Czech Republic*  
*(1) Institute of Physics, (2) Institute of Thermomechanics*

The problem of determining the ground states of atoms and lightweight molecules requires finding the lowest eigenpairs of the stationary Schroedinger equation. With heavier elements, letting aside the unsurmountable challenge of breaking the Dirac description, the real-space pseudopotential method proposed by Vackar may be used. In this work, the governing system of partial differential equations is solved by the finite element method and the characteristic eigenvalue problem by the subspace iteration method. To this end, multipurpose finite element code PMD has been adapted. The simplest test examples have been solved so far: a particle in the box problem, two particles interaction and the hydrogen atom spectrum simulation, all of them discussed in the present paper.

Key words: Schroedinger equation, finite element method, real space, pseudopotential method

## **Quantum-mechanical and continuum modelling of multiwall carbon nanotubes**

Antonio DiCarlo (1), Michele Monteferrante (1), Paolo Podio-Guidugli (2), Luciano Teresi (1)

*(1) Università degli Studi 'Roma Tre', (2) Università di Roma TorVergata, Italy*

In recent years, individual multiwall carbon nanotubes have been incorporated in various nanoelectromechanical devices of similar design, and subjected to twisting cycles either to serve as torsional oscillators [1,2], or to produce rotor bearings [3,4]. Typical length scales are: 1 micron for the overall span, 25 nm for the diameter, 0.5 nm for the interwall gap, 0.1 nm for the C-C bond length. Characteristic time scales are even more scattered. As a consequence, a multiphysics analysis is called for, combining quantum techniques with innovative applications of continuum mechanics.

The experimental evidence collected so far points out a need for a better understanding of the interwall mechanical coupling mechanisms. We speculate that the basic mechanism behind progressive interwall coupling is the formation of bridging defects, that is, covalent links between adjacent walls, produced by inward migration of in-wall defects, triggered by successive twisting cycles. Primitive defects in the outer wall are thought to be created by the interaction of Cr atoms with the C lattice structure: chromium is evaporated onto the nanotube when fabricating the device.

We propose a continuum theory of twisted MWCNTs, in which defect populations of different sorts evolve and interact with one another. The model's parameters are tuned by importing both data measured on devices and numerical results from electronic structure calculations. DFT-based studies of the energy landscape of a 2D-periodic cell comprising one or two graphite planes plus a Cr atom or dimer are carried out. The formation energies and migration barriers for several Cr configurations on both perfect and defective carbon surfaces are calculated.

Key words: NEMS; Electronic structure; Continuum mechanics.

## **Complex network modelling of soil pore architecture**

Marko Samec (1), Dean Korošak (2) and Sacha Jon Mooney (3)

*(1) Faculty of Civil Engineering, University of Maribor, Slovenia, (2) Center for Applied Mathematics and Theoretical Physics, University of Maribor, Slovenia and (3) University of Nottingham, UK*

Understanding the transport mechanisms associated with water and solutes into complex porous systems, like soils, is crucial for addressing a number of key environmental issues. Advances in research of complex systems indicate that many of them could be described as complex networks sharing a similar, underlying scale-free topological structure. In addition, recent computer simulations of random walk dynamics in such scale-free networks have parity with systems exhibiting anomalous diffusion transport properties. In this work we present the quantification of porous architecture of soils geometrically surveyed using X-ray Computed Tomography (CT). We show that pore connectivity in soils exhibits properties of the scale-free network by obtaining the power-law degree distribution. We discuss the statistical properties of the network model and implications for the macroscopic transport parameters, such as the time dependent diffusion coefficient, crucial in pore network models for the prediction of water flow and particle dynamics across a number of scales.

## **Radiating effect of participating media in a flameless industrial reactor**

Giuliano Cammarata, Giuseppe Petrone, Luca Romano

*Department of Industrial and Mechanical Engineering, University of Catania, Italy*

A numerical 3D model of a flameless reactor (50 MW) is presented in this communication. The analysed device exploits a recent combustion technique, defined as flameless oxidation, that seems to largely hinder thermal NO<sub>x</sub> formation. The functional principle of the “flameless” technology consists in using a diluted mixing of high preheating incoming fluids with exhaust inert gases before burning. The high temperature of the re-circulated combustion products is used to initiate and then to maintain a gradual oxidation throughout the volume of the combustion chamber. Due to the presence of opaque gases, radiation becomes the predominant way of heat exchange. This provides an homogeneous temperature distribution avoiding peaks of temperature, one of the cause of thermal NO<sub>x</sub> generation. In this study both fluid-dynamical and thermo-chemical behaviour of the reactor are analysed. Modelling and computations are carried-out by using a multi-physical FEM commercial software on a 64 bit platform. The fluid-dynamics of the process is based on a k-e turbulence model, coupled with four diffusion-transport equations whose the first one characterises the temperature, while the remaining three are related to the concentrations of the chemical species involving in the process. In order to consider the absorbing/emitting media contribution in the energy equation, the Rosseland approximation is invoked. Results principally highlight the relevant radiating effect on the internal heat transfer related to the presence of the gaseous participating media. As predicted by experimental data, a flat temperature profile (about 2000 K) characterises the thermal distribution throughout the entire volume of the reactor.

Key words: Numerical simulation, participating media

## **3D modeling of thermal convection in industrial Czochralski-like configurations**

D Vizman

*Physics Faculty, West University of Timisoara, Romania*

With increasing size of crystals grown by Czochralski method, the melt volumes and the corresponding crucible diameters have to increase as well. Time-dependent phenomena in the large scale melts induced by natural and forced convection due to crucible and crystal rotation are still not well understood. Improvement of numerical tools allows examining extensive parameters sets in a shorter time, which facilitates a considerable reduction of development costs. It is the aim of this talk to present how a three-dimensional simulation can describe the melt convection in industrial Czochralski-like configurations. A comparison between a Czochralski configuration for growth of Si-crystals and a Liquid Encapsulated Czochralski configuration for growth of GaAs-crystals will be done. It will be shown that higher crucible rotation rates will increase the amplitude of temperature fluctuations under the solid-liquid interface. Furthermore, the use of steady magnetic fields will be discussed as one possible way to control the convective heat transport inside the melt and therefore the interface shape.

# **Impact and Explosions**

FRIDAY 15 DECEMBER 2006  
15:30 - 17:00

CHAIR:

Z. Ren  
University of Maribor  
Slovenia

## **Impact Biomechanics of the Abdominal cavity and abdominal injury criteria**

Iztok Ciglarič, Sanid Emšo, Hermann Steffan  
*Graz University of Technology, Austria*

Currently there is no consumer or legislative guidelines that can be used to assess abdominal injuries related to car accidents. Although there is some research results and data related to abdominal impact biomechanics and injuries further investigation is necessary. The European Commissions 6<sup>th</sup> framework collaborative project, APROSYS (Advanced Protective Systems) has a subproject titled "Biomechanics" that initiates advanced research in the field of human impact biomechanics. As a part of this subproject Graz University of Technology studies abdominal biomechanics and abdominal injury criteria. To cope with this problem Graz University of Technology investigated real life car accident cases related to abdominal injuries. Further Graz University of Technology perform series of tests on volunteers and cadavers. Also complex numerical model of abdominal cavity was developed and studied by using HUMOS2 human body model. Abdominal numerical model was validated by using experimental data. For a selected load cases we perform numerical analysis to assess abdominal loads and possible injuries. New injury criteria for abdominal cavity were suggested.

## **Composite under impact loading**

P R Hampson, M Moatamedi  
*University of Salford, Manchester, UK*

An extensive literature review of composite impact work has been conducted which summarised key research interests and provided an overview of the development of theoretical, experimental and numerical methods for low, high, and hyper velocity impact. Particular attention was given to the experimental apparatus and techniques used for the different impact velocity regimes, and the implementation of failure criteria in finite element (FE) modelling methods which are used to predict material behaviour. Areas were then identified for which limited research had been undertaken and suggestions were made for possible future research topics. To date, validation exercises using examples taken from published literature for metal/metal and metal/composite impact have been undertaken to determine if the numerical techniques used in the FE software ANSYS/LS-DYNA accurately represents the transient dynamic response of projectile impacts. An instrumented low velocity impact rig has also been constructed to acquire experimental data for comparison with numerical results. Future work will involve the construction of a shock tube to subject composite test specimens to air blast loading. These experimental results will then be compared with numerical solutions.

Keywords: Composites, Impact behaviour, Failure criterion, Finite Element

## **On mechanism of non-heating sterilization using the underwater shock wave loading and gas-formation**

A Takemoto (1), M Otsuka (2), Y Mibuka (3), M Iwahara (4), S Itoh (1)  
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In the field that can't use apply thermal sterilization, the establishment of the sterilization technology with non-heating is strongly requested. Hence, the underwater shock wave loading caused by explosive was used for non-heating sterilization.

*Saccharomyces cerevisiae* was used for experiments. *S. cerevisiae* starts fermentation by feeding the glucose, and causes CO<sub>2</sub> within its body. There is the great density difference between cells of *S. cerevisiae* and the gas, therefore, a strong reflected wave is caused on the boundary of the cell and the gas, and a remarkable expansion is caused. Fermented *S. cerevisiae* showed high sterilization rates and non-fermented showed low sterilization rates.

The sterilization rate on three conditions was as follows in the order of higher. 1) Fermenting, high pressure. 2) Fermenting, low pressure. 3) Non-fermenting, high pressure.

The detonation fuse is used in this experiment. There was an interesting phenomenon, that is, the sterilization rate is high at the side of detonation beginning, and it is lowering toward the direction. It is thought that this is related to keeping of a constant angle. A corresponding result to the phenomenon was gotten by the numerical analysis about the progress and the end of the detonation and pressure.

Key words: Underwater Shock Wave, Non-heating Sterilization, Numerical Analysis

## **Verification of numerical dispersion analysis by a two cylinders impact problem**

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In terms of wave propagation analysis, discrete structures behave like band-pass filters with discontinuity between individual frequency bands. Analogous appearances occur in modelling of nonstationary problems in solid continuum mechanics by means of the finite element method (FEM). Spatial discretization of a continuum introduces dispersion error to a numerical solution of wave propagation. Despite of many papers published on the subject, little attention has been paid so far to higher-order elements. Belytschko and Mullen (1978) were the first to extend the dispersion analysis to quadratic one-dimensional finite elements. The dispersion study of the three-dimensional second-order Helmholtz equation was carried out by Abbound and Pinsky (1992) for 20-node elements. However, the dispersion analysis of a standard solid mechanics problem has not yet been performed. In this work, the numerical dispersion of two-dimensional finite elements is studied including the effects of spatial and time discretization. The outcome of this dispersion study was verified by the analytical solution to the longitudinal impact of two cylindrical bars as derived by Vales et al. (1996). The analytical solution is quite complicated expressing the distribution of displacements and stresses in the form of an infinite series of improper integrals. In accordance with the results of the dispersion analysis it was proved that the quadratic elements showed better accuracy than the linear ones.

Key words: FEM, wave propagation, dispersion, quadratic elements

## **Numerical Simulation of a metal sheet during explosive forming**

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It has been difficult to effectively and accurately form materials, such as aluminium based alloys, using conventional methods. Recently, explosive forming with a capability of producing larger deformations than is possible with normal static press forming has become an interesting research topic and is seen as an alternative to traditional methods. However, when the affecting pressure wave is too large, the metal sheet may be destroyed. Explosive forming using under water shockwaves is examined in this research paper through both experiment and numerical simulation. The explosive forming was performed using the free stretch forming method, allowing a better understanding of the basic mechanisms and characteristics. Numerical simulations are performed in three dimensions using the LS-DYNA code. Experimental and numerical results are seen to correspond to a high degree.

Key words: explosive forming, underwater shock wave, numerical simulation





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