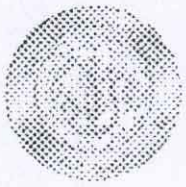


ANSCSE 13

13th Annual Symposium on Computational Science and Engineer (ANSCSE13)

March 25 – 27, 2009, Faculty of Engineer, Kasetsart University, Bangkok, Thailand

March 2, 2009

Acceptance Letter for ANSCSE13

Dear Yee Siew Choong,

We are pleased to inform you that the submission of your scientific contribution (Abstract ID 265) titled "Elucidating Isoniazid Resistance in *Mycobacterium tuberculosis* Enoyl-acyl Carrier Protein Reductase"

by First Author: Yee Siew Choong
Others Authors: Habibah A. Wahab

is accepted for presentation in ANSCSE13. Please visit ANSCSE13 website for the registration and mode information. (http://www.hpcnc.com/anscse13)

We look forward to your participation in ANSCSE13 in March 2009.

Department of Computer Engineering, Faculty of Engineering, Kasetsart University, Bangkok, Thailand. 10900
Tel: 02-9428555 ext 1403, 1404, Fax: 02-5796245
E-mail: pu@ku.ac.th, secretary@hpcnc.com

ANSCSE 13

13th ANnual Symposium on Computational Science and Engineering

March 25-27, 2009

Kasetsart University
Bangkok, THAILAND

Message from Chairman of ANSCSE 13

Dear Colleagues and Friends,

Welcome to ANSCSE 13!

Computational Science and Engineering becomes one of a rapid growing areas in term of the significant and community size. Many new and innovative high performance computing platform, algorithm, and software enable scientists to explore even deeper into the wonder of nature around us. Computational techniques have been applied to create many new and exciting things such as new break-through drug, deeper understanding about life at the genetic and molecular level, design of new engineering product that is cheaper, safer, and faster. In Thailand, Computational Science and Engineering has been practiced by so many groups for so many years.

Thus, it is my great pleasure that Department of Chemistry, and Department of Computer Engineering, Kasetsart University (KU) are jointly organizing 13th ANnual Symposium on Computational Science and Engineering (ANSCSE 13) from March 25 – 27, 2009, at Faculty of Engineering, Kasetsart University, Bangkok, Thailand. ANSCSE 13 is a great forum of leading computational scientists in Thailand and many countries around the world. We are very exciting that conference covers many interesting areas of computation science and engineering disciplines such as Computational Physics, Computational Chemistry, Computational Biology and Bioinformatics, Computation Fluid Dynamics and Solid Mechanics, HPC and Grid computing, Computer Science and Engineering and Computational Mathematics. Eminent scientists have been invited to present the Plenary, Keynote and Invited lectures in ANSCSE 13.

In summary, ANSCSE 13 is really become a landmark event that mark the state of the development of computational area in Thailand. I wish that every participant will enjoy the intellectual exchange that takes place during the conference. Finally, I wish you success in pushing forward the state of the art in your area and hope that we will meet each other again next year.

Message from Chairperson of Scientific Program Committee

Kasetsart University is delighted and proud to be honored by the Computational Science and Engineering Association as the co-host in organizing 13th ANnual Symposium on Computational Science and Engineering (ANSCSE 13). The conference has been held during March 25-27, 2009, at Kasetsart University, Bangkok, Thailand.

As of Conference Scientific Program, ANSCSE 13 has invited eminent scientists with 3 plenary lectures and 11 invited lectures come from 6 countries. Also, the Computational Network Consortium (CNC) of NANOTEC and NECTEC meeting and a Special Workshop on Introduction to GPU Computing Technology by HPCNC are organized. We were very delighted that ANSCSE13 has 110 presentations and 200 participants. Furthermore, the conference has also initiated to award Outstanding Paper.

The conference offered a scientific program that covered recent and advanced researches on broad range of topics in the field of Computational Physics, Computational Chemistry, Computational Biology and Bioinformatics, Computation Fluid Dynamics and Solid Mechanics, HPC and Grid computing, Computer Science and Engineering and Computational Mathematics, Industrial Tracks, Special session for Graduate Students and meeting with CFD speakers.

I would like to take this opportunity to convey my special thanks to all contributed papers all committees, consultants, especially the academic committees for reviewing contributed papers, and the conference secretariats who have been working extremely hard to make this conference a success.

Supa Hannongbua
Chairperson, ANSCSE 13 Scientific Committee
Department of Chemistry, Faculty of Science, Kasetsart University

Message from President of Computational Science and Engineering Association

Welcome to Kasetsart University and to the 13th ANnual Symposium on Computational Science and Engineering (ANSCSE 13). This is the first ANSCSE organized by the Computational Science and Engineering Association (CSEA); the previous ANSCSE has been co-organized by universities and National Electronics and Computer Technology Center (NECTEC). Since the first ANSCSE in 1997, our computational science and engineering (CSE) research network has continued to grow and strengthen such that we could form our association in September 2007. CSEA should become a new center of CSE research collaboration, and, co-organizing ANSCSE with universities and research institutes has been adopted as a main activity.

An objective of ANSCSE is to serve as a stage to train new generations of CSE researchers. ANSCSE is a chance for them to present their works, so that they can experience an essential part of research profession, that is to share their findings by making presentation and publication, and, to be appraised by peers. So, I would like to encourage our young participants to take this opportunity to exchange ideas with friends from different research groups and even from different research areas as well as different countries.

ANSCSE also serves as an informal forum for collaboration among CSE researchers. CSE is a good tool to facilitate interdisciplinary collaborations. At the same time, CSE also benefits from interdisciplinary collaborations. Therefore, we have tried to design the program to allow generous time for interactions of researchers, scientists and engineers among the same field and across different fields. We also have poster and demonstration exhibition from research groups, institutes and industrial companies. We have received generosity from many respectable scientists and engineers to participate as keynote and invited speakers. I strongly believe that direct interaction with them will stimulate a lot of new research ideas among us.

CSEA is a newly established association. Our aim is to support and facilitate research, education and collaboration among researchers and research institutes across the fields of CSE. As CSE researchers, you should find the association beneficial to our CSE research community. CSEA will not only be the center for collaborations within our community, but it will also be the contact point to other research community and the general public. I hope to welcome you as CSEA new members. You can find more information about how you can participate in CSEA in this symposium and on our website.

To this end, I appreciate the keynote, plenary and invited lecturers as well as other participants who contributed to the conference, particularly those from oversea. I take the opportunity to thank the steering committees, the program committees and the organizing committees who have worked hard for the success of ANSCSE 13. I also thank Kasetsart University, NECTEC and other sponsors for their generous supports.

I wish ANSCSE 13 a fruitful success, and hope that all of you enjoy the sharing and exchanging of your expertise.

Supa Hannongbua
President of Computational Science and Engineering Association (CSEA)

PROGRAM SUMMARY

Wednesday, March 25, 2009

Time	Room 0410 Building 14
08.30 - 09.00	Registration
09.00 - 09.20	Opening Ceremony
9.00	-Report by ANSCSE13 Chairman
9.05	-Welcome address by Dean of Faculty of Engineering
9.10	-Opening Speech by the President of Kasetsart University
09.20 - 09.50	**KEYNOTE LECTURE** Chairman: **Putchong Uthayopas** (Kasetsart University, Thailand) **Sakarindr Bhumiratana** (NSTDA Director, Thailand) **"NSTDA Strategic direction for National S&T Development and some applications of Computational Science and Engineering"**
09.50 - 10.25	**PLENARY LECTURE I** Chairman: **Putchong Uthayopas** (Kasetsart University, Thailand) **Takayuki Aoki** (Tokyo Institute of Technology, Japan) **"Remarkable Speed-up of CFD Applications by GPU Computing"**
10.25 - 11.00	Coffee Break
11.00 - 12.00	Oral Presentation (5 parallel sessions)

Room 202	*Room 203*	*Room 204*	*Room 503*	*Room 507*
Computational Physics (I)	***Computational Chemistry (I)***	***Computational Fluid Dynamics and Solid Mechanics (I)***	***HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (I)***	***Industrial Track (I)***
• INV-1 • S1-OR1 • S1-OR2	• INV-2 • S2-OR1 • S2-OR2	• INV-3 • S3-OR1 • S3-OR2	• S4-OR1 • S4-OR2 • S4-OR3 • S4-OR4	• Technology update from IBM • Technology update from Microsoft

12.00 - 13.30	LUNCH
13.30 - 14.50	Oral Presentation (5 parallel sessions)

Room 202	*Room 203*	*Room 204*	*Room 503*	*Room 507*
Computational Physics (II)	***Computational Chemistry (II)***	***Computational Fluid Dynamics and Solid Mechanics (II)***	***HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (II)***	***Computational Biology and Bioinformatics (I)***
• S1-OR3 • S1-OR4 • S1-OR5 • S1-OR6 • S1-OR7	• INV-4 • S2-OR3 • S2-OR4 • S2-OR5 • S2-OR6	• S3-OR3 • S3-OR4 • S3-OR5 • S3-OR6 • S3-OR7	• S4-OR5 • S4-OR6 • S4-OR7 • S4-OR8	• INV-5 • S5-OR1 • S5-OR2 • S5-OR3

14.50 - 15.20	Coffee Break

PROGRAM SUMMARY

	Room 202	*Room 203*	*Room 204*	*Room 503*	*Room 507*
15.20 - 16.40	• S1-OR8 • S1-OR9 • S1-OR10 • S1-OR11 • S1-OR12	• INV-6 • S2-OR7 • S2-OR8 • S2-OR9 • S2-OR10	• S3-OR8 • S3-OR9 • S3-OR10 • S3-OR11	• S4-OR9 • S4-OR10 • S4-OR11 • S4-OR12 • S4-OR13	• INV-7 • S5-OR4 • S5-OR5 • S5-OR6
17.00 - 19.00	WELCOME PARTY				

Thursday, March 26, 2009

Time	*Room 0410 Building 14*
08.30 - 09.00	Registration
09.00 - 09.35	**PLENARY LECTURE II** Chairperson: **Supa Hannongbua** (Kasetsart University, Thailand) **Habibah A Wahab** (University Sains Malaysia, Malaysia) **"Overcoming Challenges in Natural Product Discovery through Informatics and Computational Approaches"**
09.35 - 10.10	**PLENARY LECTURE III** Chairman: **Ekachai Juntasaro** (King Mongkut's University of Technology North Bangkok, Thailand) **Tamer Zaki** (Imperial College London, England) **"Direct numerical simulations of continuous and discrete mode interactions, and breakdown to turbulence"**
10.10 - 10.40	Coffee Break
10.40 - 12.10	Oral Presentation (5 parallel sessions)

Computer Engineering Building (Building 15)

Room 202	*Room 203*	*Room 204*	*Room 503*	*Room 507*
Computational Physics (III)	***Computational Chemistry (III)***	***Computational Fluid Dynamics and Solid Mechanics (III)***	***HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (III)***	***Industrial Track (II)***
• INV-8 • S1-OR13 • S1-OR14 • S1-OR15 • S1-OR16	• INV-9 • S2-OR11 • S2-OR12 • S2-OR13 • S2-OR14	• S3-OR12 • S3-OR13 • S3-OR14 • S3-OR15	• S4-OR14 • S4-OR15 • S4-OR16 • S4-OR17	• Technology update from Intel • Technology update from ChemoInformatics

12.10 - 13.30	LUNCH
13.30 - 14.50	Oral Presentation (5 parallel sessions)

Room 202	*Room 203*	*Room 404*	*Room 503*	*Room 507*
Computational Physics (IV)	***Computational Chemistry (IV)***	***Computational Fluid Dynamics and Solid Mechanics (IV)***	***HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (IV)***	***Computational Biology and Bioinformatics (II)***
• S1-OR17 • S1-OR18 • S1-OR19	• INV-10 • S2-OR15 • S2-OR16 • S2-OR17 • S2-OR18	Meet the CFD speakers round table	• S4-OR18 • S4-OR19 • S4-OR20 • S4-OR21	• INV-11 • S5-OR7 • S5-OR8 • S2-OR24 • S2-OR25

14.50 - 15.20	Coffee Break				
	Room 202	*Room 203*	*Room 404*	*Room 503*	*Room 507*
15.20 - 16.40	***Special session for Graduate Students***	• S2-OR19 • S2-OR20	TBA	• S4-OR22 • S4-OR23	***Industrial Track (III)***
	• S6-OR1 • S6-OR2 • S6-OR3 • S6-OR4 • S6-OR5	• S2-OR21 • S2-OR22 • S2-OR23		• S4-OR24	• Direct Implementation Skill in Top 3 Computer Cluster of Thailand." by Cluster Kit
17.00-19.00	CLOSING CEREMONY at Room 202				

Friday, March 27, 2009

Time	*Computer Engineering Building (Building 15)*	
	Room 201	*Room 202*
09.00 - 12.00	***HPC workshop***	***Computation Network Consortium (CNC) Workshop***
	Introduction to GPU Computing Technology By HPCNC team (Putchong Uthayopas, KU)	CNC workshop By Sornthep Vannarat (NECTEC) and Yuthana Tantirungrotechai (NANOTEC) • Introduction to CNC Project • CNC software tool
12:00 - 13:30	LUNCH	
13:30 - 16:30	Windows Clustering Technology by INOX	TBA

Remark: TBA = To be assigned

Invited Lecturers

INV-1 "Computational Challenges and Progress in Cosmology"
Grant Mathews, University of Notre Dame, USA

INV-2 "Photochemistry of Biological Chemosensor, Organic Light-Emitting Diodes, and Inner-shell Electronic Processes"
Masahiro Ehara, Institute for Molecular Science, Japan

INV-3 "Next-generation High Performance Computing for Catalytic Reactions on Metal Surface: Strategy and Design"
Kei Kuramoto, University of Hyogo, Japan

INV-4 "Toward Absolute Reaction Rate Theory In Solution Via Free Energy Gradient Method With Extensive Molecular Dynamics Simulations"
Masataka NAGAOKA, Nagoya University, Japan

INV-5 "Deriving Protein Dynamical Properties from Weighted Protein Contact Number"
Jenn-Kang HWANG, National Chiao Tung University, Taiwan

INV-6 "Theoretical Investigation on the Structures and Photoionizations of Quintuply-Bonded Dichromium Complexes"
Jen-Shiang K. Yu, National Chiao Tung University, Taiwan

INV-7 "Protein folding and aggregation: an antagonistic reaction of spontaneous folding and diffusion limited aggregation"
Chia-Ching Chang, National Chiao Tung University, Taiwan

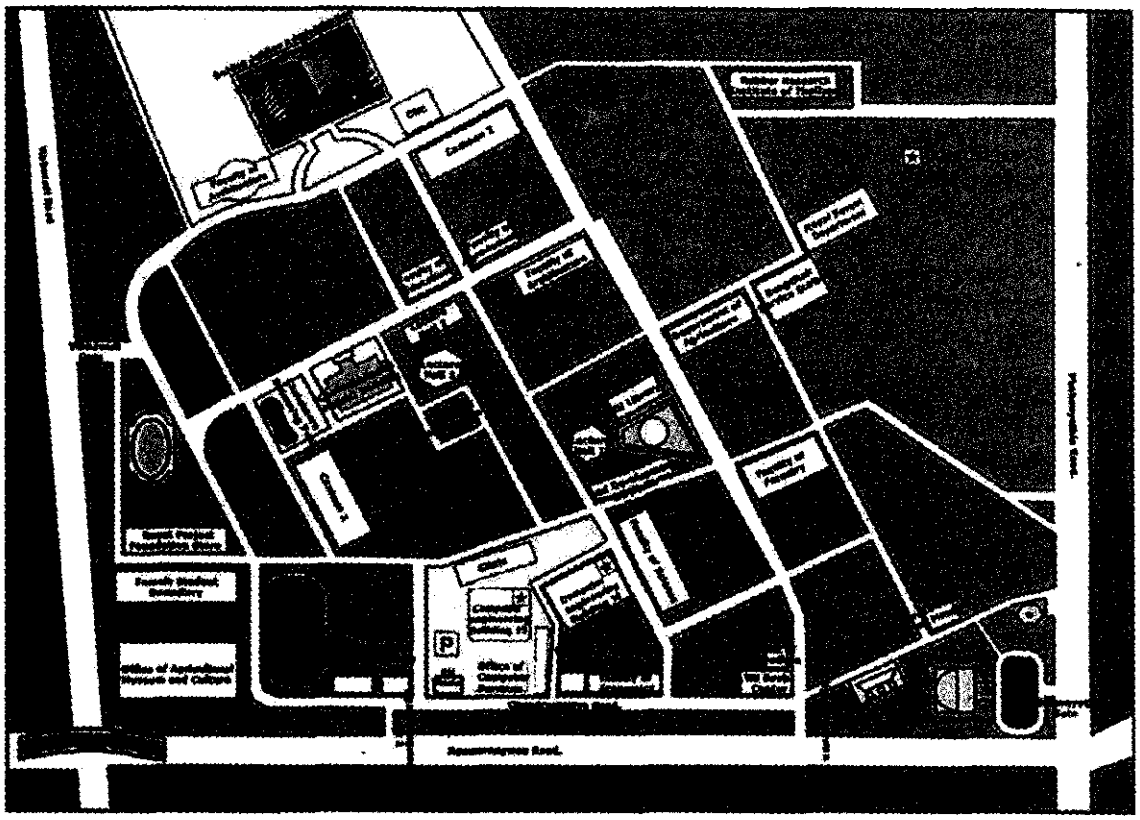
INV-8 "Crystal phase transformations under specific loading conditions"
Sukit Limpijumnong, Suranaree University of Technology, Thailand

INV-9 "QM/MM calculations in drug discovery: A useful method for studying binding phenomena?"
Paul Gleeson, GlaxoSmithKline Company, USA

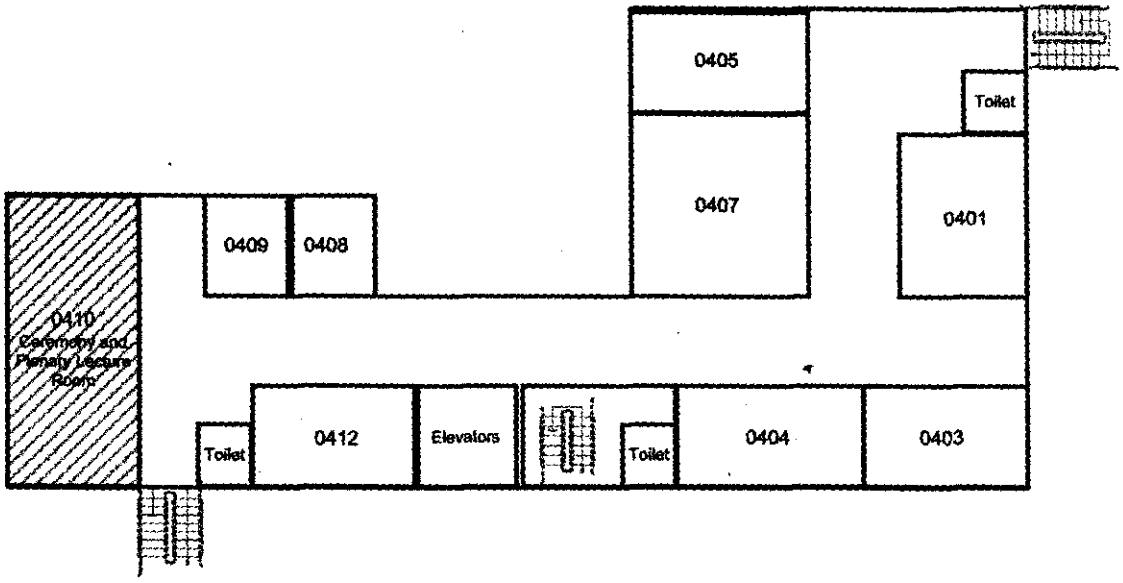
INV-10 "Structural determination of ions solvated in aqueous electrolyte solutions: A combined X-ray absorption near-edge structure (XANES) experiments and QM/MM MD-based simulations study"
Anan Tongraar, Suranaree University of Technology, Thailand

INV-11 "Predicting Complexation Thermodynamics Parameters of β -Cyclodextrin with Enantiomeric Pairs of Chiral Guest by using Swarm Intelligence and Support Vector Machines"
Luckhana Lawtrakul, Sirindhorn International Institute of Technology, Thailand

The Conference Center Map

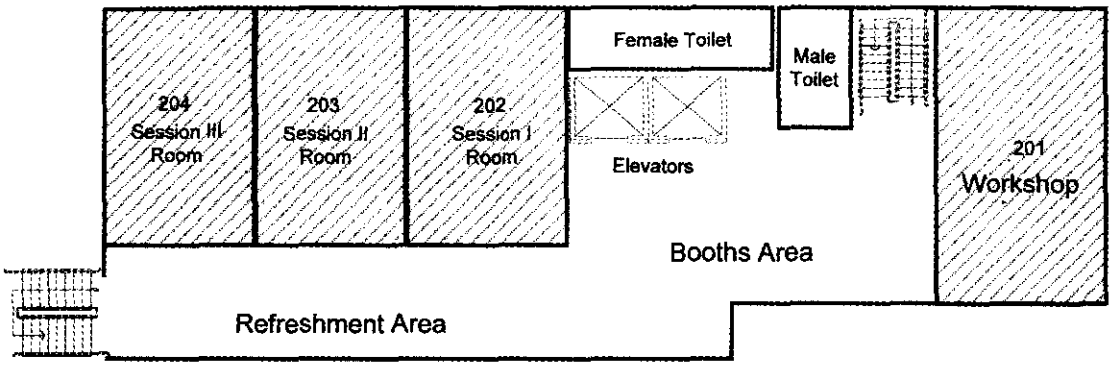


Building 14 Floor 4

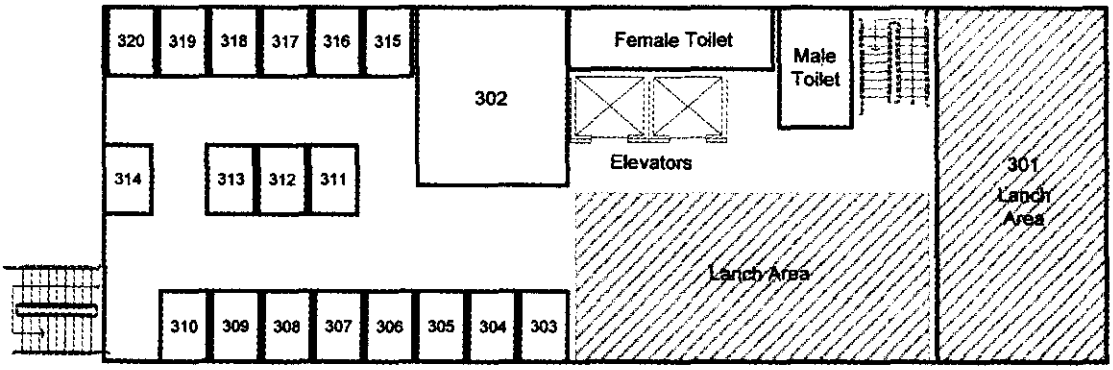


The Conference Center Map

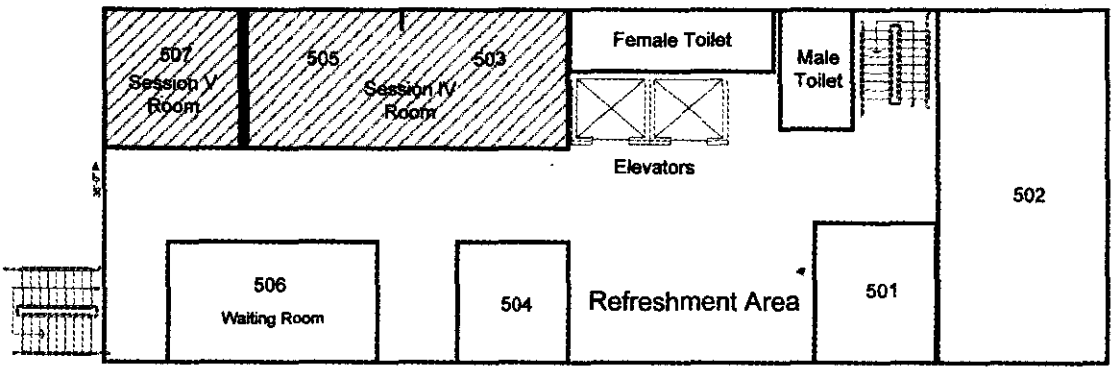
Building 15 Floor 2



Building 15 Floor 3



Building 15 Floor 5



Oral Presentation Schedule

Computer Engineering Building (Building 15), Faculty of Engineering		
S1- Computational Physics		
March 25, 2009		
Room 202	**Chairman:** David Ruffolo (MU)	
11.00 – 11.30	INV-1	**Grant Mathews** (University of Notre Dame, USA), "Computational Challenges and Progress in Cosmology"
11.30-11.45	S1-OR1	**Piyanate Chuychai**, "Diffusion of Charged Particles in Isotropic Magnetic Turbulence"
11.45-12.00	S1-OR2	**Tawat Rung-Arunwan**, "Domain Decomposition for 2D Magnetotelluric Forward Modeling"
12.00-13.30	Lunch	
Room 202	**Chairman:** Anucha Yangthaisong (UBU)	
13.30-13.45	S1-OR3	**Lee Sin Ang**, "Spin Contamination in the Hartree-Fock and MP2 Wave functions of Graphene"
13.45-14.00	S1-OR4	**Surakarn Thitianan**, "The Development of Automated Plasma Parameters Analytic Algorithm for Electrical Probe Measurement"
14.00-14.15	S1-OR5	**Panida Lorwongtragool**, "Computational Studies on the Dynamics and Trajectories of Li^+ Intercalated into Single-Walled Carbon Nanotube"
14.15-14.30	S1-OR6	**Jaturong Sukonthachat**, "The 1st Order Ordinary Differential Equation for Producing a 3D Real Image by Visible Light"
14.30-14.45	S1-OR7	**Abdulmutta Thatribud**, "First-principles Computation of ferroelectricity in $Pb(Zr_xTi_{1-x})O_3$ Superlattices"
14.50-15.20	Coffee Break	
Room 202	**Chairman:** Yongyut Laosiritaworn (CMU)	
15.20-15.35	S1-OR8	**Pranuda Jivaganont**, "Improved Performance in Planar Anode-Supported Solid Oxide Fuel Cell"
15.35-15.50	S1-OR9	**Watcharawuth Krittinatham**, "Drift Motions of Energetic Protons in an Interplanetary Magnetic Cloud"
15.50-16.05	S1-OR10	**Pat Wongpan**, "Field Line Random Walk Simulation in Arbitrarily Stretched Isotropic Turbulence"
16.05-16.20	S1-OR11	**Achara Seripienlert**, "Local Trapping Boundaries, Current Sheets, and Their Roles for Dropout Features"
16.20-16.35	S1-OR12	**Puwis Amatyakul** , "Joint Inversion of 2-D Direct-Current Resistivity (DCR) and Magnetotelluric (MT) data: DASOCC algorithm"
March 26, 2009		
Room 202	**Chairman:** Anucha Yangthaisong (UBU)	
10.40 -11.10	INV-8	**Sukit Limpijumnong** (Suranaree University of Technology, Thailand), "Crystal Phase Transformations under Specific Loading Conditions"
11.10-11.25	S1-OR13	**Gjindara Wong-ud-dee**, "Analysis of Effect of Temperature on Mechanical and Thermophysical Properties of $SrTiO_3$ by Molecular Dynamics Method"
11.25-11.40	S1-OR14	**Tosawat Seetawan**, "Molecular Orbital Calculations of n and p-types Thermoelectric Oxide Material by the DV-Xα Method"
11.40-11.55	S1-OR15	**Anuwat Boonthummo**, "*Ab Initio* Study in Physical Properties of $(X_xFe_{1-x})Se$ pnictide Compounds"
11.55-12.10	S1-OR16	**Noparit Jinuntuya**, "Elementary Excitations of the Bimodal Ising Spin Glass on a Square Lattice"
12.10-13.30	Lunch	
Room 202	**Chairman:** Tosawat Seetawan (SNRU)	
13.30-13.45	S1-OR17	**Areeya Chantasri**, "Percolation of Loose Bonds Using Spin-Correlation Functions of the Bimodal 2-Dimensional Ising Spin Glass"
13.45-14.00	S1-OR18	**Krisda Sudprasert**, "Investigating Non-Equilibrium Statistical Mechanics of a Driven Lattice Gas"
14.00-14.15	S1-OR19	**Watchareeya Chairatch**, "Studies of the Electronic and Optical Properties of $BaTiO_3$ and $CaCu_3Ti_4O_{12}$ Using First Principles Calculations"

Oral Presentation Schedule

S2 – Computational Chemistry		
March 25, 2009		
Room 203	**Chairman**: Vudhichai Parasuk (CU)	
11.00-11.30	**INV-2**	**Masahiro Ehara** (Institute for Molecular Science, Japan), "Photochemistry of Biological Chemosensor, Organic Light-Emitting Diodes, and Inner-shell Electronic Processes"
11.30-11.45	S2-OR1	**S. B. Pongsai**, "Hydrogen Storage Improved by Embedding Metal Atoms in Zeolite Extra-Framework"
11.45-12.00	S2-OR2	**Pirada Sudprasert**, "Loading Distribution of Isoamyl Acetate in Zeolite"
12.00-13.30	Lunch	
Room 203	**Chairman**: Anan Tongraar (SUT)	
13.30-14.00	**INV-4**	**Masataka NAGAOKA** (Nagoya University, Japan), "Toward Absolute Reaction Rate Theory In Solution Via Free Energy Gradient Method With Extensive Molecular Dynamics Simulations"
14.00-14.15	S2-OR3	**Oraphan Saengsawang**, "Diffusion of *n*-pentane in Zeolite ZK5 Studied by HTCE and Transition Path Sampling"
14.15-14.30	S2-OR4	**Kanjarat Sukrat**, "Transition State of Proton Exchange and Degradation Reactions of Ethane and Propane in ZSM-5 Zeolite"
14.30-14.45	S2-OR5	**Tanawut Ploymeerusmee**, "Molecular Dynamic Simulations of Carbon Dioxide in MOF-5"
14.45-15.00	S2-OR6	**Janchai Yana**, "Theoretical Study of Effect of Ar^+ Bombardment on Nafion Side Chain"
14.50-15.20	Coffee Break	
Room 203	**Chairperson**: Duangkamol Gleeson (KMITL)	
15.20-15.35	**INV-6**	**Jeu-Shiang K. Yu** (National Chiao Tung University, Taiwan), "Theoretical Investigation on the Structures and Photoionizations of Quintuply-Bonded Dichromium Complexes"
15.35-15.50	S2-OR7	**Uthumporn Arsawang**, "Structure and Binding Energy of GEMZAR® Encapsulated in Functionalized Carbon Nanotube"
15.50-16.05	S2-OR8	**Purinchaya Sornmee**, "Molecular Dynamics Study of Encapsulation of Doxorubicin Inside Single-Walled Carbon Nanotube"
16.05-16.20	S2-OR9	**Atichat Wongkoblap**, "Effects of Functional Group on Adsorption of Water in Carbon Nanotube Bundles: Computer Simulation and Experimental Studies"
16.20-16.35	S2-OR10	**Arthit Vongachariya**, "Effects of Tube Diameter and Boron-Nitrogen Doping on Electronic Band Structure of Single-Walled Carbon Nanotubes"
March 26, 2009		
Room 203	**Chairman**: Piti Treesukol (KU)	
10.40-11.10	**INV-9**	**Paul Gleeson** (GlaxoSmithKline Company, USA), "QM/MM calculations in drug discovery: A useful method for studying binding phenomena?"
11.10-11.25	S2-OR11	**Panita Decha**, "Determinants of Substrate Specificity of Furin on the Inserted Sequences of High Pathogenic H5N1 Hemagglutinin: a MD Study"
11.25-11.40	S2-OR12	**Nopphorn Kaiyawet**, "Recognition of Hemagglutinin in Avian Influenza Virus to Human Sialic-Galactose Using *in silico* Technique"
11.40-11.55	S2-OR13	**Thanyarat Udommaneethanakit**, "MD/LIE Free Energy of Ligand Binding to N1 Neuraminidase of Avian Influenza A (H5N1) Virus"
11.55-12.10	S2-OR14	**Pathumwadee Intharathep**, "Allosteric Interaction between an Rimantadine Drug and the Influenza A M2 Protein Channel in Phospholipid Studied by MD Simulations"
12.10-13.30	Lunch	
Room 203	**Chairman**: Waraporn Parasuk (KU)	
13.30-14.00	**INV-10**	**Anan Tongraar** (Suranaree University of Technology, Thailand), "Structural Determination of Ions Solvated in Aqueous Electrolyte Solutions: A Combined X-Ray Absorption Near-Edge Structure (XANES) Experiments and QM/MM MD-based Simulations Study"

Oral Presentation Schedule

14.00-14.15	S2-OR15	**Naser Eltaher Eltayeb**, "Synthesis, Characterization and Luminescence Properties of Aqua{5,5'-dihydroxy-2,2'-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato-κ^4O,N,N',O'}zinc(II): Experimental and Theoretical Study Towards Organic Light Emitting Diodes"
14.15-14.30	S2-OR16	**Thanisorn Yakhantip**, "Theoretical Studies of Carbazole Fluorene Derivatives As organic dye molecules use in Dye-Sensitized Solar Cells (DSSCs)"
14.30-14.45	S2-OR17	**Ruangchai Tarsang**, "Structural, Electronic and Optical Properties of the Perylene Derivatives for Application in Dye-Sensitized Solar Cells (DSSCs) Based on TD-DFT Investigation"
14.45-15.00	S2-OR18	**Tatiya Chokbunpiam**, "Structural and Electronic Properties of Porphyrin-Thiophene-Perylene Compound As Studied by Quantum Chemical Calculations"
15.00-15.20	Coffee break	
Room 203	**Chairman**: Pipat Kongpracha (KU)	
15.20-15.35	S2-OR19	**Wathang Donkrajang**, "Study of Interactions between Metalloporphyrins with Various Volatile Substances Using Computational Quantum Mechanics and Molecular Dynamics Simulations"
15.35-15.50	S2-OR20	**Panthip Tue-ngeun**, "Pairwise Decomposition of Residue Interaction Energies of Single Chain Fv Antibody and its Peptide Epitopes"
15.50-16.05	S2-OR21	**Darinee Sae-Tang**, "Effect of Water Molecule in Cyclopropane Synthase Cofactor Binding Site by Quantum Chemical Calculations"
16.05-16.20	S2-OR22	**Poonsiri Thipnate**, "QSAR Analysis for Cytotoxicity of Lamellarins Against Human Hormone-Dependent 747D Breast Cancer Cells"
16.20-16.35	S2-OR23	**Waraporn Jungtanasombut**, "QSAR of Soil Organic Partition Coefficient of Benzene Derivatives"

S3- Computational Fluid Dynamics and Solid Mechanics

March 25, 2009

Room 204	**Chairman**: Sirod Sirisup (NECTEC)	
11.00-11.30	**INV-3**	**Kei Kuramoto** (University of Hyogo, Japan), "Next-generation High Performance Computing for Catalytic Reactions on Metal Surface: Strategy and Design"
11.30-11.45	S3-OR1	**Thanarak Srisurat**, "Computational Fluid Dynamics Studies of Multi-tubular Wall Coated Reactor for Methane Steam Reforming"
11.45-12.00	S3-OR2	**Winit Jaiboon**, "Simulation of Flow Aerodynamics and Heat Transfer in a Plate-fin Radiator"
12.00-13.30	Lunch	
Room 204	**Chairman**: Vejapong Juttijudata (KU)	
13.30-13.45	S3-OR3	**Sirod Sirisup**, "Reduced-order Modeling of Forced Convective Heat Transfer with Time-Dependent Boundary Conditions"
13.45-14.00	S3-OR4	**Bumroong Puangkird**, "Pressure-Drop and Extensional Rheology Extracted from the Numerical Computations of Viscoelastic Flows in Cross-Slot Devices"
14.00-14.15	S3-OR5	**Prachakon Kaewkhiaw**, "Simulation of Cavitation on a Marine Propeller using CFD"
14.15-14.30	S3-OR6	**Pikul Puphasuk**, "Two Rigid Spheres in Low-Reynolds-Number Gradient Flow"
14.30-14.45	S3-OR7	**Nattapon Chantarapanich**, "Stress Distributions in Knees after Open Wedge High Tibial Osteotomy: A Finite Element Study"
14.50-15.20	Coffee break	
Room 204	**Chairman**: Varangrat Juntasaro (KU)	
15.20-15.35	S3-OR8	**Jakgrit Sompong**, "A Numerical Study of the Flow and Heat Transfer Around two Rotating Circular Cylinders in Side-by-side Arrangements"
15.35-15.50	S3-OR9	**Saifhon Tomkratoke**, "Three-dimensional Direct Numerical Simulation of Mixed Convection Heat Transfer in Square Enclosure"
15.50-16.05	S3-OR10	**Folfon Srisawat**, "The Effect of Velocity on the Vibration of Motorcycle Mirror"
16.05-16.20	S3-OR11	**Patipat Puttong**, "Effects from Blood Flow on Heat Transfer During Cancer Treatment using Hyperthermia Method"

March 26, 2009		
Room 204	**Chairman**: Nikolay Moshkin (SUT)	
10.40-11.10	S3-OR12	**Piyawut Kaewrit**, "The Evaluation of Turbulence Model on Two-Phase Flow Inside Complex Flock Cabinet"
11.10-11.25	S3-OR13	**Kridsada Narong**, "On the Performance of High-Resolution Advection Schemes in the Context of Laminar Mixed Region Collapse in Density Stratified Fluid"
11.25-11.40	S3-OR14	**Teerawoot Lomlai**, "Molecular Dynamics Simulation of Surface Roughness Effect in a Nanochannel"
11.40-11.55	S3-OR15	**Pairin Suwannasri**, "Numerical Simulation of the Fluid Flow Past a Torus"

S4 – HPC and Grid computing, Computer Science and Engineering and Computational Mathematics

March 25, 2009		
Room 503	**Chairman**: Vara Varavithya (KMUTNB)	
11.00-11.15	S4-OR1	**Khongthep Boonmee**, "The Develpment of a Framework for Performance Analysis of Parallel Programs"
11.15-11.30	S4-OR2	**Phithak Thaenkaew**, "A Framework for Centralized Authentication and Account Management on Large-Scale Cluster Environment"
11.30-11.45	S4-OR3	**Narapat Saengpatsa**, "Improving Scalability and Fault Tolerance of Open MPI Using Binomial Graph Topology"
11.45-12.00	S4-OR4	**Rakpong Kaewpuang**, "High performance Parallel Applications for Pickup and Delivery Problem with Time Window on Multicore System"
12.00-13.30	Lunch	
Room 503	**Chairman**: Putchong Uthayopas (KU)	
13.30-13.45	S4-OR5	**Sedtha Pota**, "Recognition of Altitude Numeric of Index Contour Lines from Scanned Topographic Maps Using Density Based Clustering and Back- propagation Neural Network Techniques"
13.45-14.00	S4-OR6	**Kalyamol Saelao**, "Horizontal Orientation Motion Capture Using Neural Network"
14.00-14.15	S4-OR7	**Chakrawal Ariyasaranee**, "ECG Classification Using Weightless Neural Networks with Synaptic Optimization"
14.15-14.30	S4-OR8	**Udomsak Chirabandit**, "Mel Based on Octave Spectral Histogram in Music Genre Classification Using Neural Networks"
14.50-15.20	Coffee Break	
Room 503	**Chairman**: Sornthep Vannarat (NECTEC)	
15.20-15.35	S4-OR9	**Anuchit Jitpattanakul**, "An Algorithm for Learning *k*-DFA from Informant"
15.35-15.50	S4-OR10	**Ekaphon Monthonjulaket**, "Subtraction Algorithm for The Double-Base Number System"
15.50-16.05	S4-OR11	**K. Suranga Kahatadeniya**, "An Ant Colony Optimization Algorithm for Slope Stability Analysis of Multilayer Solis"
16.05-16.20	S4-OR12	**Kanon Sujaree**, "A Max-Min Ant System Algorithm for Cell Formation Problem"
16.20-16.35	S4-OR13	**Pakon Thuphairo**, "A Design of Asynchronous Double Grain Reconfigurable Computing Array"
March 26, 2009		
Room 503	**Chairman**: Vara Varavithya (KMUTNB)	
10.40-10.55	S4-OR14	**Angkoon Phinyomark**, "Evaluation of Mother Wavelet Based on Robust EMG Feature Extraction Using Wavelet Packet Transform"
10.55-11.10	S4-OR15	**Wongnaret Khantuwan**, "Improving Voronoi Generator Points Detection Using Local Polygon Adaptation"
11.10-11.25	S4-OR16	**Khammapun Khantanapoka**, "A Simulation Study of Pattern Three Dimension Free-from in the Complex Level"
11.25-11.40	S4-OR17	**Wiboon Kuenghakit**, "Applied Fisher Linear Discrimination to Recognize the Multi-view Shape based on Multi-level Triangle Area Representation"
12.10-13.30	Lunch	

Oral Presentation Schedule

Room 503	**Chairman**: Putchong Uthayopas (KU)	
13.30-13.45	S4-OR18	**Somrerk Poodchakarn**, "LVDTs Measurement Computation for Tilting and Misalignment of Sheet Metal Forming Tool"
13.45-14.00	S4-OR19	**Songpon Klinchaeam**, "Condition Monitoring of a Small four Stroke Petrol Engine Using Statistical Covariance Parameter Analysis"
14.00-14.15	S4-OR20	**Songkran Siridejachai**, "A Numerical Study of the Waveguide Length Affects Power Distribution Inside the Microwave Oven"
14.15-14.30	S4-OR21	**Wongyos Keardsri**, "Defining Privacy Levels for IP Address Anonymization"
14.50-15.20	Coffee Break	
Room 503	**Chairman**: Somthep Vannarat (NECTEC)	
15.20-15.35	S4-OR22	**Wongyos Keardsri**, "Presenting Privacy Tree Structure for IP Address Anonymization Based on Privacy Levels"
15.35-15.50	S4-OR23	**Prataru Chotipanbandit**, "An Information Hiding Model for Intelligent Audio Watermarking"
15.50-16.05	S4-OR24	**Nittaya Kerdprasop**, "Higher-Order Logic Programming and the Development of Association Miner"

S5 – Computational Biology and Bioinformatics

March 25, 2009

Room 507	**Chairman**: Jeerayut Chaijaruwanich (CMU)	
13.30-14.00	**INV-5**	**Jenn-Kang HWANG** (National Chiao Tung University, Taiwan), "Deriving Protein Dynamical Properties from Weighted Protein Contact Number"
14.00-14.15	S5-OR1	**Wichian Sittiprapaporn**, "Preattentive Processing of Synthesized Complex Sounds Perception in the Human Brain: Microstate Segmentation and Low-Resolution Electromagnetic Tomography (LORETA) Studies"
14.15-14.30	S5-OR2	**Angkoon Phinyomark**, "A Novel EMG Feature Extraction For Tolernace of Interference"
14.30-14.45	S5-OR3	**Thanika Seephueak**, "Searching for Genetic Factors from Different Variation Patterns of Gene Expression Microarray Data"
14.50-15-20	Coffee Break	
Room 507	**Chairman**: Krisana Waiyamai (KU)	
15.20-15.50	**INV-7**	**Chia-Ching Chang** (National Chiao Tung University, Taiwan), "Protein Folding and Aggregation: An Antagonistic Reaction of Spontaneous Folding and Diffusion Limited Aaggregation"
15.50-16.05	S5-OR4	**Narumol Doungpan**, "On the Integrative Analysis of Network-based Biomarkers of Autism Spectrum Disorder from Gene Expression Profiles and Protein-Protein Interaction Network"
16.05-16.20	S5-OR5	**Patcharaporn Sereejaitham**, "Multilevel Quality Control in Pooled-DNA Genome Wide Association Study of Osteoporosis"
16.20-16.35	S5-OR6	**Wassana Munkong**, "A Constraint-Based Boolean Approach to Inferring Genetic Circuits"

March 26, 2009

Room 507	**Chairperson**: Luckhana Lawtrakul (SIIT), Patchreenart Saparpakorn (KU)	
13.30-14.00	**INV-1 1**	**Luckhana Lawtrakul** (Sirindhorn International Institute of Technology, Thailand), "Predicting Complexation Thermodynamics Parameters of β -Cyclodextrin with Enantiomeric Pairs of Chiral Guest by using Swarm Intelligence and Support Vector Machines"
14.00-14.15	S5-OR7	**Piyachat Udomwong**, "Prediction of ABA Responsive Genes in Rice Genome Based on *cis*-Regulatory Elements Using Conditional Random Fields Method"
14.15-14.30	S5-OR8	**Konrapob Klaywong**, "Virtual Screening for antiviral drugs against RNA-Binding Domain of Non-structural (NS1) Protein of Avian Influenza Virus A"
14.30-14.45	S2-OR24	**Auradee Punkvang**, "Insight into the Binding Interactions of Arylamides as the Direct Inhibitors of Enoyl ACP Reductase from *Mycobacterium Tuberculosis*, Using Molecular Docking, Quantum Chemical Calculations and 3D-QSAR Studies"
14.45-15.00	S2-OR25	**Patchreenart Saparpakorn**, "CoMFA Study of 2-Aminopyrimidin-4(3H)-ones as Potent NNRTIs"

Oral Presentation Schedule

S6 - Special session for Graduate Students		
March 26, 2009		
Room 202	**Chairman**: Chak Sangma (KU)	
15.20-15.35	S6-OR1	**Wai Keat Yam**, "Elucidating Macrolide Binding Pocket in 50S Ribosomal Subunit Using Molecular Dynamics Simulation"
15.35-15.50	S6-OR2	**Thipvaree Wangchareansak**, "Host Type Selectivity Prediction for Birdflu Virus"
15.50-16.05	S6-OR3	**Yee Siew Choong**, "Elucidating Isoniazid Resistance in *Mycobacterium tuberculosis* Enoyl-acyl Carrier Protein Reductase"
16.05-16.20	S6-OR4	**Krongkaew Navakul**, "Effect of Antigenic Site Mutation on Cell Receptor Binding of Influenza A virus (H5N1) Hemagglutinin"
16.20-16.35	S6-OR5	**Sy Bing Choi**, "Sequence Analysis and Molecular Docking Simulation Approaches to Predict the Function of Hypothetical Protein from *Klebsiella Pneuomoniae*"

Abstract Content

Plenary lecture

Invited Lecture

Computational Physics

Computational Chemistry

Abstract Content

Computation Fluid Dynamics and Solid Mechanics

Abstract Content

Abstract Content

HPC and Grid computing, Computer Science and Engineering and Computational Mathematics