PERPUSTAKAAN KAMPUS KESIHATAN UNIVERSITI SAINS MALAYSIA

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ANSCEE 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.

Yours sincerely,

Putchong Uthayopas Chairman, ANSCSE13 Local Organizing Committee Faculty of Engineering, Kasetsart University, Bangkok, Thailand

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

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.

Putchong Uthayopas Chairman, ANSCSE 13 Local Organizing Committee Faculty of Engineering, Kasetsart University

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.

Lupa Hannongburg

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.

Super Hannongburg

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

PROGRAM SUMMARY

Wednesday, March 25, 2009

18.58 CON 198 CON 18 1				Koon	0410 Building 14
08.30 - 09.00	Registration				
9.00 - 09.20	Opening Ceremony				
9.00	-Report by ANSCSE13	Chairman			
9.05	-Welcome address by I	Dean of Faculty of Engine	cring		
9.10	-Opening Speech by the	e President of Kasetsart U	niversity		۰.
09.20 - 09.50	KEYNOTE LECTUR	E			
	Chairman; Putchong U	J thayopas (Kasetsart Univ	versity, Thailand)		
		ns (NSTDA Director, Th			
		-		oplications of Computational	Science and
09.50 - 10.25	PLENARY LECTUR	EI			
	Chairman: Putchong U	J thayopas (Ka setsart Uni	versity, Thailand)		
	Takayaki Aoki (Toky	o Institute of Technology,	Japan)		
	"Remarkable Speed-u	up of CFD Applications l	by GPU Computing"		
10.25 - 11.00	Coffee Break				
1.00 - 12.00	Oral Presentation (5 pa	rallel sessions)			
	Room 202	Room 203	Room 204	Room 503	Room 507
	Room 202 Computational Physics (I)	Room 203 Computational Chemistry (I)	Room 204 Computational Fluid Dynamics and Solid Mechanics (I)	HPC and Grid Computing, Computer Science and Engineering and Computational	Room 507 Industrial Track (I)
	Computational Physics (1) • INV-1	Computational Chemistry (I) • INV-2	Computational Fluid Dynamics and Solid Mechanics (I) • INV-3	HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (1) • S4-OR1	Industrial Track (1) Technology
	Computational Physics (1)	Computational Chemistry (I)	Computational Fluid Dynamics and Solid Mechanics (I)	HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (1)	Industrial Track (1)
12.00 - 13.30	Computational Physics (1) • INV-1 • S1-OR1	Computational Chemistry (I) • INV-2 • \$2-OR1	Computational Fluid Dynamics and Solid Mechanics (I) • INV-3 • S3-OR1	HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (1) • S4-OR1 • S4-OR2 • S4-OR3	Industrial Track (1) Technology update from IBM Technology update from
12.00 - 13.30 13.30 - 14.50	Computational Physics (1) • INV-1 • S1-OR1 • S1-OR2	Computational Chemistry (J) • INV-2 • S2-OR1 • S2-OR2	Computational Fluid Dynamics and Solid Mechanics (I) • INV-3 • S3-OR1	HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (1) • S4-OR1 • S4-OR2 • S4-OR3	Industrial Track (I) Technology update from IBM Technology update from
the second	Computational Physics (1) • INV-1 • S1-OR1 • S1-OR2 LUNCH	Computational Chemistry (J) • INV-2 • S2-OR1 • S2-OR2	Computational Fluid Dynamics and Solid Mechanics (I) • INV-3 • S3-OR1	HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (1) • S4-OR1 • S4-OR2 • S4-OR3 • S4-OR4	Industrial Track (1) Technology update from IBM Technology update from
t de la	Computational Physics (1) • INV-1 • S1-OR1 • S1-OR2 LUNCH Oral Presentation (5 pa	Computational Chemistry (1) • INV-2 • S2-OR1 • S2-OR2	Computational Fluid Dynamics and Solid Mechanics (I) • INV-3 • S3-OR1 • S3-OR2	HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (1) • S4-OR1 • S4-OR2 • S4-OR3 • S4-OR3 • S4-OR4	Industrial Track (1) Technology update from IBM Technology update from Microsoft
t de la	Computational Physics (1) • INV-1 • S1-OR1 • S1-OR2 LUNCH Oral Presentation (5 pa Room 202 Computational Physics (11) • S1-OR3	Computational Chemistry (I) • INV-2 • S2-OR1 • S2-OR2 trallel sessions) Room 203 Computational Chemistry (II) • INV-4	Computational Fluid Dynamics and Solid Mechanics (I) • INV-3 • S3-OR1 • S3-OR2 Room 204 Computational Fluid Dynamics and Solid Mechanics (II) • S3-OR3	HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (1) • S4-OR1 • S4-OR2 • S4-OR3 • S4-OR3 • S4-OR4	Industrial Track (1) Technology update from IBM Technology update from Microsoft Room 507 Computational Biology and Biology and Bioinformatics (1) INV-5
1. de 1. de	Computational Physics (1) • INV-1 • S1-OR1 • S1-OR2 LUNCH Oral Presentation (5 pa Room 202 Computational Physics (11) • S1-OR3 • S1-OR4	Computational Chemistry (I) INV-2 S2-OR1 S2-OR2 rallel sessions) Room 203 Computational Chemistry (II) INV-4 S2-OR3	Computational Fluid Dynamics and Solid Mechanics (I) INV-3 S3-OR1 S3-OR2 Room 204 Computational Fluid Dynamics and Solid Mechanics (II) S3-OR3 S3-OR4	HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (1) • S4-OR1 • S4-OR2 • S4-OR3 • S4-OR3 • S4-OR4 <i>Room 503</i> HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (11) • S4-OR5 • S4-OR6	Industrial Track (1) Technology update from IBM Technology update from Microsoft Room 507 Computational Biology and Bioinformatics (1) INV-5 S5-OR1
t de la	Computational Physics (1) • INV-1 • S1-OR1 • S1-OR2 LUNCH Oral Presentation (5 pa Room 202 Computational Physics (11) • S1-OR3 • S1-OR4 • S1-OR5	Computational Chemistry (I) • INV-2 • S2-OR1 • S2-OR2 rallel sessions) Room 203 Computational Chemistry (II) • INV-4 • S2-OR3 • S2-OR4	Computational Fluid Dynamics and Solid Mechanics (I) • INV-3 • S3-OR1 • S3-OR2 Room 204 Computational Fluid Dynamics and Solid Mechanics (II) • S3-OR3 • S3-OR4 • S3-OR5	HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (1) • S4-OR1 • S4-OR2 • S4-OR3 • S4-OR3 • S4-OR4 • S4-OR4 • S4-OR4 • S4-OR4 • S4-OR4 • S4-OR5 • S4-OR5 • S4-OR5 • S4-OR5 • S4-OR7	Industrial Track (1) Technology update from IBM Technology update from Microsoft Room 507 Computational Biology and Biology and Bioinformatics (1) INV-5 S5-OR1 S5-OR1 S5-OR2
t de la	Computational Physics (1) • INV-1 • S1-OR1 • S1-OR2 LUNCH Oral Presentation (5 pa Room 202 Computational Physics (11) • S1-OR3 • S1-OR4	Computational Chemistry (I) INV-2 S2-OR1 S2-OR2 rallel sessions) Room 203 Computational Chemistry (II) INV-4 S2-OR3	Computational Fluid Dynamics and Solid Mechanics (I) INV-3 S3-OR1 S3-OR2 Room 204 Computational Fluid Dynamics and Solid Mechanics (II) S3-OR3 S3-OR4	HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (1) • S4-OR1 • S4-OR2 • S4-OR3 • S4-OR3 • S4-OR4 <i>Room 503</i> HPC and Grid Computing, Computer Science and Engineering and Computational Mathematics (11) • S4-OR5 • S4-OR6	Industrial Track (1) Technology update from IBM Technology update from Microsoft Room 507 Computational Biology and Bioinformatics (1) INV-5 S5-OR1

PROGRAM SUMMARY

1444	Room 202	Room 203	Room 204	Room 503	Room 507
15.20 - 16.40	• S1-OR8	• INV-6	• S3-OR8	• S4-OR9	• INV-7
	• S1-OR9	• S2-OR7	• S3-OR9	• S4-OR10	 S5-OR4
	• S1-OR10	• S2-OR8 ·	• S3-OR10	• S4-OR11	• S5-OR5
	• S1-OR11	• S2-OR9	• S3-OR11	• S4-OR12	• S5-OR6
	• S1-OR12	 S2-OR10 		• S4-OR13	

Thursday, March 26, 2009

Time				Room	0410 Building 14	
08.30 - 09.00	Registration					
09.00 - 09.35	PLENARY LECTUR	RE II				
	Chairperson: Supa H	annongbua (Kasetsart Un	iversity, Thailand)			
	Habibah A Wahab (University Sains Malaysia	, Malaysia)			
	"Overcoming Challe	nges in Natural Product	Discovery through Informat	tics and Computational App	roaches"	
09.35 - 10.10	PLENARY LECTUR	RE III				
07.50 10.10			s University of Technology N	orth Bangkok Thailand)		
				orui Dangkok, Thanand)		
		l College London, England				
	"Direct numerical sin	mulations of continuous a	and discrete mode interactio	ns, and breakdown to turbu	lence"	
10.10 - 10.40	Coffee Break					
10.40 - 12.10	Oral Presentation (5 p		puter Engineering Building (I	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	• INV-9	• \$3-OR12	• S4-OR14	Technology	
	 S1-OR13 S1-OR14 	 S2-OR11 S2-OR12 	S3-OR13S3-OR14	S4-OR15S4-OR16	update from Intel Technology	
	S1-OR15S1-OR16	 S2-OR13 S2-OR14 	• S3-OR15	• S4-OR17	update from ChemoInformatics	
10.10 10.00		1 02-0114		*		
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	• INV-10	Meet the CFD speakers round table	• S4-OR18	• INV-11	
	S1-OR18S1-OR19	S2-OR15S2-OR16	Tourid table	S4-OR19S4-OR20	S5-OR7S5-OR8	
		S2-OR17S2-OR18		• S4-OR21	S2-OR24S2-OR25	
		· 52-0K18	*		• 52-0K25	

PROGRAM SUMMARY

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 		S4-OR22 S4-OR23	Industrial Track (III)	
	• S6-OR1	• S2-OR21	TBA	• S4-OR24	Direct	
	 S6-OR2 S6-OR3 	 S2-OR22 S2-OR23 			Implementation Skill in Top 3	
	• \$6-OR4				Computer Cluster of Thailand." by	
	• S6-OR5				Cluster Kit	
17.00-19.00	CLOSING CEREMO	NY 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

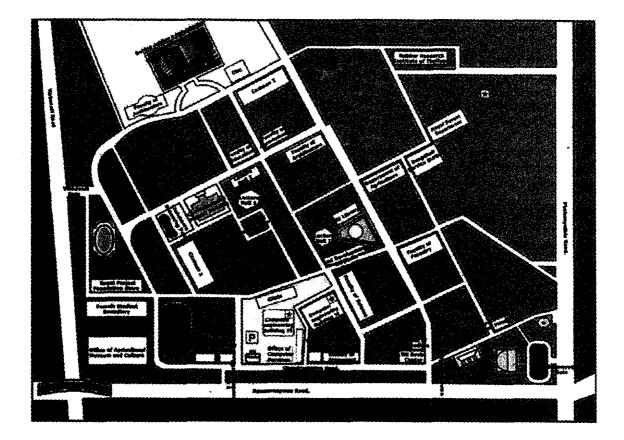
INV-8 "Crystal phase transformations under specific loading conditions" Sukit Limpijumnong, Suranaree University of Technology, Thailand

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

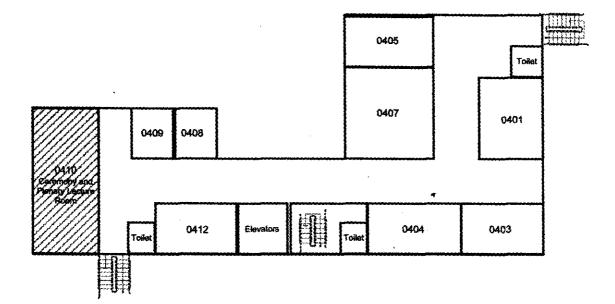
INV-10 "Structural determination of ions solvated in aqueous electrolyte solutions: A combined X-ray absorption near-edge structure (XANES) experiments and QM/MM MD-based simulations study" Anan Tongraar, Suranaree University of Technology, Thailand

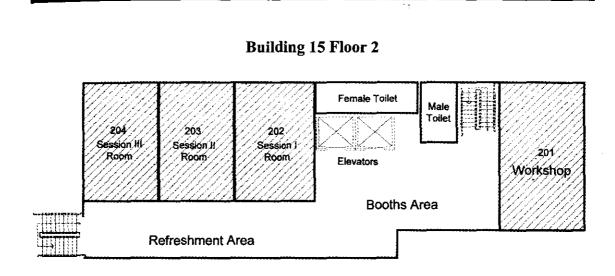
INV-11 "Predicting Complexation Thermodynamics Parameters of β-Cyclodextrin with Enantiomeric Pairs of Chiral Guest by using Swarm Intelligence and Support Vector Machines" Luckhana Lawtrakul, Sirindhorn International Institute of Technology, Thailand

The Conference Center Map



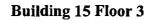
Building 14 Floor 4

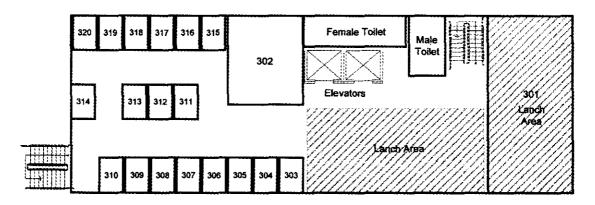




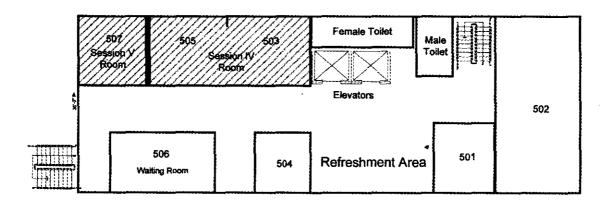
The Conference Center Map

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Building 15 Floor 5



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Compu	ter Engineering Building (Building 15), Faculty of Engineering
ational Phy	sics
	March 25, 2009
Chairman: J	David Ruffolo (MU)
INV-1	Grant Mathews (University of Notre Dame, USA), "Computational Challenges and Progress in
	Cosmology"
SI-ORI	Piyanate Chuychal, "Diffusion of Charged Particles in Isotropic Magnetic Turbulence"
S1-OR2	Tawat Rung-Arunwan, "Domain Decomposition for 2D Magnetotelluric Forward Modeling"
Lunch	<u>.</u>
Chairman:	Anucha Yangthaisong (UBU)
SI-OR3	Lee Sin Ang, "Spin Contamination in the Hartree-Fock and MP2 Wave functions of Graphene"
SI-OR4	Surakarn Thitianan, "The Development of Automated Plasma Parameters Analytic Algorithm for
	Electrical Probe Measurement"
SI-OR5	Panida Lorwongtragool, "Computational Studies on the Dynamics and Trajectories of Li ⁺
	Intercalated into Single-Walled Carbon Nanotube"
S1-OR6	Jaturong Sukonthachat, "The 1* Order Ordinary Differential Equation for Producing a 3D Real
	Image by Visible Light"
\$1-OR7	Abdulmutta Thatribud, "First-principles Computation of ferroelectricity in Pb(Zr _x Ti _{1-x})O ₃
}	Superlattices"
Coffee Break	۲
Chairman	Yongyut Lausinitawom (CMU)
S1-OR8	Pranuda Jivaganout, "Improved Performance in Planar Anode-Supported Solid Oxide Fuel Cell"
SI-OR9	Watcharawuth Krittinatham, "Drift Motions of Energetic Protons in an Interplanetary Magnetic
1	Cloud"
S1-OR10	Pat Wongpan, "Field Line Random Walk Simulation in Arbitrarily Stretched Isotropic Turbulence"
S1-OR11	Achara Seripienlert, "Local Trapping Boundaries, Current Sheets, and Their Roles for Dropout
	Features"
SI-OR12	Puwis Amatyakul, "Joint Inversion of 2-D Direct-Current Resistivity (DCR) and Magnetotelluric
	(MT) data: DASOCC algorithm"
	March 26, 2009
(Chilymony)	Anucha Yangthansong (17813)
INV-8	Sukit Limpijumnong (Suranaree University of Technology, Thailand), "Crystal Phase
{ ·	Transformations under Specific Loading Conditions"
SI-OR13	Gjindara Wong-ud-dee, "Analysis of Effect of Temperature on Mechanical and Thermophysical
	Properties of SrTiO ₃ by Molecular Dynamics Method"
SI-OR14	Tosawat Sectawan, "Molecular Orbital Calculations of n and p-types Thermoelectric Oxide Material
	by the DV-Xa Method"
SI-OR15	Anuwat Boonthummo, "Ab Initio Study in Physical Properties of (XxFe1.x)Se pnictide Compounds"
S1-OR16	Noparit Jinuntuya, "Elementary Excitations of the Bimodal Ising Spin Glass on a Square Lattice"
Lunch	***************************************
Chaleman:	Topawat Sectawan (SMRU)
SI-ORI7	Areeya Chantasri, "Percolation of Loose Bonds Using Spin-Correlation Functions of the Bimodal 2
	Dimensional Ising Spin Glass"
S1-OR18	Krisda Sudprasert, "Investigating Non-Equilibrium Statistical Mechanics of a Driven Lattice Gas"
(
S1-OR19	Watchareeya Chairatch, "Studies of the Electronic and Optical Properties of BaTiO3 and
	ational Phy Chairman: INV-1 SI-OR1 SI-OR2 Lunch Chairman SI-OR3 SI-OR3 SI-OR3 SI-OR5 SI-OR5 SI-OR7 Coffee Breal Chairman SI-OR8 SI-OR7 Coffee Breal SI-OR7 SI-OR7 Coffee Breal SI-OR7 SI-OR7 SI-OR7 SI-OR7 SI-OR7 SI-OR7 SI-OR7 SI-OR7 SI-OR7 SI-OR7 SI-OR7 SI-OR7 SI-OR7 SI-OR10 SI-OR11 SI-OR11 SI-OR13 SI-OR13 SI-OR13 SI-OR14 SI-OR15 SI-OR17

II.00-II.30 INV-2 II.00-II.30 INV-2 II.30-II.45 S2-OR II.45-I2.00 S2-OR I2.00-I3.30 Lunch Room 203 Chairma I3.30-I4.00 INV-4 I4.00-I4.15 S2-OR I4.15-I4.30 S2-OR I4.30-I4.45 S2-OR I4.30-I4.45 S2-OR I4.30-I4.45 S2-OR I4.50-I5.20 Coffee B Room 203 Chairpe I5.20-I5.35 INV-6 I5.35-I5.50 S2-OR I5.50-I6.05 S2-OR I6.05-I6.20 S2-OR I6.20-I6.35 S2-OR I6.20-I6.35 S2-OR I0.40-I1.10 INV-5 I1.10-I1.25 S2-OR I1.25-I1.40 S2-OR I1.40-I1.55 S2-OR I1.55-I2.10 S2-OR	Framework" Pirada Sudprasert, "Loading Distribution of Isoamyl Acetate in Zeolite" m: Anan Tongraar (SUT) Masataka NAGAOKA (Nagoya University, Japan), "Toward Absolute Reaction Rate Theory In Solution Via Free Energy Gradient Method With Extensive Molecular Dynamics Simulations" Oraphan Saengsawang, "Diffusion of n-pentane in Zeolite ZK5 Studied by HTCE and Transition Path Sampling" Kanjarat Sukrat, "Transition State of Proton Exchange and Degradation Reactions of Ethane and Propane in ZSM-5 Zeolite" Tanawut Ploymeerusmee, "Molecular Dynamic Simulations of Carbon Dioxide in MOF-5"
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Room 203 Chairpe 15.20-15.35 INV-6 15.35-15.50 S2-OR 15.50-16.05 S2-OR 16.05-16.20 S2-OR 16.05-16.20 S2-OR 16.05-16.20 S2-OR 16.20-16.35 S2-OR 10.40-11.10 INV-5 11.10-11.25 S2-OR 11.25-11.40 S2-OR 11.40-11.55 S2-OR 11.55-12.10 S2-OR	
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15.50-16.05 S2-OR 16.05-16.20 S2-OR 16.20-16.35 S2-OR 16.20-16.35 S2-OR 16.20-16.35 S2-OR 10.40-11.10 INV-5 11.10-11.25 S2-OR 11.25-11.40 S2-OR 11.40-11.55 S2-OR 11.55-12.10 S2-OR	Structures and Photoionizations of Quintuply-Bonded Dichromium Complexes"
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16.05-16.20 S2-OR 16.20-16.35 S2-OR 16.20-16.35 S2-OR 16.20-16.35 S2-OR 10.40-11.10 INV-5 11.10-11.25 S2-OR 11.25-11.40 S2-OR 11.40-11.55 S2-OR 11.55-12.10 S2-OR	Functionalized Carbon Nanotube"
I6.20-16.35 S2-OR1 Room 203 Chairman 10.40-11.10 INV-5 11.10-11.25 S2-OR1 11.25-11.40 S2-OR1 11.40-11.55 S2-OR1 11.55-12.10 S2-OR1	Purinchaya Sornmee, "Molecular Dynamics Study of Encapsulation of Doxorubicin Inside Single-
I6.20-16.35 S2-OR1 Room 203 Chairman 10.40-11.10 INV-5 11.10-11.25 S2-OR1 11.25-11.40 S2-OR1 11.40-11.55 S2-OR1 11.55-12.10 S2-OR1	Walled Carbon Nanotube"
Room 203 Chairman 10.40-11.10 INV-5 11.10-11.25 S2-OR 11.25-11.40 S2-OR 11.40-11.55 S2-OR 11.55-12.10 S2-OR	Atichat Wongkoblap, "Effects of Functional Group on Adsorption of Water in Carbon Nanotube
Room 203 Chairman 10.40-11.10 INV-5 11.10-11.25 S2-OR 11.25-11.40 S2-OR 11.40-11.55 S2-OR 11.55-12.10 S2-OR	Bundles: Computer Simulation and Experimental Studies"
10.40-11.10 INV-5 11.10-11.25 S2-OR1 11.25-11.40 S2-OR1 11.40-11.55 S2-OR1 11.55-12.10 S2-OR1	0 Arthit Vongachariya, "Effects of Tube Diameter and Boron-Nitrogen Doping on Electronic Band
10.40-11.10 INV-5 11.10-11.25 S2-OR1 11.25-11.40 S2-OR1 11.40-11.55 S2-OR1 11.55-12.10 S2-OR1	Structure of Single-Walled Carbon Nanotubes"
10.40-11.10 INV-5 11.10-11.25 S2-OR1 11.25-11.40 S2-OR1 11.40-11.55 S2-OR1 11.55-12.10 S2-OR1	March 26, 2009
11.10-11.25 S2-OR 11.25-11.40 S2-OR 11.40-11.55 S2-OR 11.55-12.10 S2-OR	n: Piti Treesukol (KU)
11.25-11.40 S2-OR: 11.40-11.55 S2-OR: 11.55-12.10 S2-OR:	Paul Gleeson (GlaxoSmithKline Company, USA), "QM/MM calculations in drug discovery: A used
11.25-11.40 S2-OR: 11.40-11.55 S2-OR: 11.55-12.10 S2-OR:	method for studying binding phenomena?"
11.40-11.55 S2-OR 11.55-12.10 S2-OR	Panita Decha, "Determinants of Substrate Specificity of Furin on the Inserted Sequences of High
11.40-11.55 S2-OR 11.55-12.10 S2-OR	Pathogenic H5N1 Hemagglutinin: a MD Study"
11.55-12.10 S2-OR1	2 Nopphorn Kaiyawet, "Recognition of Hemagglutinin in Avian Influenza Virus to Human Sialic-
11.55-12.10 S2-OR1	Galactose Using in silico Technique"
	3 Thanyarat Udommaneethanakit, "MD/LIE Free Energy of Ligand Binding to N1 Neuraminidase
	Avian Influenza A (H5N1) Virus"
12.10-13.30 Lunch	4 Pathumwadee Intharathep, "Allosteric Interaction between an Rimantadine Drug and the Influenz
12.10-13.30 Lunch	A M2 Protein Channel in Phospholipid Studied by MD Simulations"
Room 203 Chairm	n: Warapoin Párasuk (KU)
13.30-14.00 INV-1	Anan Tongraar (Suranarce University of Technology, Thailand), "Structural Determination of Ions
	Solvated in Aqueous Electrolyte Solutions: A Combined X-Ray Absorption Near-Edge Structure

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-k ⁴ O,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: I	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
l		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- Comput	ational Flui	id 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
111-0 11:20		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
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		for Methane Steam Reforming"
11 45-12 00	\$3-OR2	for Methane Steam Reforming" Winit talkaon "Simulation of Flow Actor/gramics and Heat Transfer in a Plate-fin Radiator"
11.45-12.00	S3-OR2	for Methane Steam Reforming" Winit Jaiboon, "Simulation of Flow Aerodynamics and Heat Transfer in a Plate-fin Radiator"
12.00-13.30	Lunch	Winit jaiboon, "Simulation of Flow Aerodynamics and Heat Transfer in a Plate-fin Radiator"
12.00-13.30 Room 204	Lunch Chairman	Winit Jaiboon, "Simulation of Flow Aerodynamics and Heat Transfer in a Plate-fin Radiator" Vejapong Juttijudata (KU)
12.00-13.30	Lunch	Winit jaiboon, "Simulation of Flow Aerodynamics and Heat Transfer in a Plate-fin Radiator" Vejapong Juthijudata (KU) Sirod Sirisup, "Reduced-order Modeling of Forced Convective Heat Transfer with Time-Dependent
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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"
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		March 25, 2009
Room 503	Chairman:	Vara Varavithya (KMUTNB)
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	•	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
	4	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
	4	Optimization"
14.15-14.30	S4-OR8	Udomsak Chirabandit, "Mel Based on Octave Spectral Histogram in Music Genre Classification
	1	Using Neural Networks"
14.50-15.20	Coffee Brea	k
Room 503	Chairman:	Somthep 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	\$4-OR11	K. Suranga Kahatadeniya, "An Ant Colony Optimization Algorithm for Slope Stability Analysis of
	ļ	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"
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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
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12.10-13.30	Lunch	

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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"
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15.35-15.50	S4-OR23	Pratarn 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: J	eerayut 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	\$5-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	\$5-OR2	Angkoon Phinyomark, "A Novel EMG Feature Extraction For Tolemace of Interference"
14.30-14.45	S5-OR3	Thanika Seephueak, "Searching for Genetic Factors from Different Variation Patterns of Gene
		Expression Microarray Data"
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15.20-15.50	INV-7	Chis-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	\$5-OR6	Wassana Munkong, "A Constraint-Based Boolean Approach to Inferring Genetic Circuits"
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13.30-14.00	INV-11	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	\$2-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"

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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 <i>Mycobacterium tuberculosis</i> 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"		
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