International Symposium on Computational Science 2011

Date: February 15 – 17, 2011

Venue: Kanazawa University, Kakuma Campus, Kanazawa, Japan
Building of Natural Science and Technology,
Lecture rooms n.103 and n.104 (Feb. 15-16),
Lecture room n.301 (Feb. 17)

Organized by:

Department of Computational Science,
Faculty of Science, Kanazawa University

Faculty of Mathematics and Natural Sciences,
Bandung Institute of Technology

Organizing Committee:

K. Svadlenka (Kanazawa University)
M. Saito (Kanazawa University)
K. Nishikawa (Kanazawa University)
S. Omata (Kanazawa University)
H. Nagao (Kanazawa University)
S. Miura (Kanazawa University)
M. A. Martoprawiro (Bandung Institute of Technology)
S. Haryono (Bandung Institute of Technology)
R. Simanjuntak (Bandung Institute of Technology)
R. Hertadi (Bandung Institute of Technology)

Sponsored by:

Fujitsu Limited

JSPS Grant-in-Aid (No. 21654013, S. Omata)

Symposium Program

February 15 (Tuesday): 1st day

10:00-10:30 Registration
10:30-10:40 Opening address

Morning session (room 103, chairperson: Mineo Saito)
10:40-11:20 **Laksana Tri Handoko** (Indonesian Institute of Sciences)
Modeling nano particle dynamics using statistical mechanics approach
11:20-12:00 **Suprijadi Haryono** (Bandung Institute of Technology)
Uniaxial stress effect on crystal dislocations movement and crack propagation in cubic crystal

Lunch break

Afternoon session 1 (room 103, chairperson: Kiyoshi Nishikawa)
14:00-14:40 **Harno Pranowo** (Universitas Gadjah Mada)
Microsolvation conformation of crown ether-transition metal cation complexes by ab initio method
14:40-15:20 **Muhamad A. Martoprawiro** (Bandung Institute of Technology)
Computational study of iron(II)-based spin transition complex

Afternoon session 2 (room 104, chairperson: Karel Svadlenka)
14:00-14:40 **Shinya Okabe** (Iwate University)
The existence of shortening-straightening flow for non-closed planar curves with infinite length
14:40-15:20 **Hideki Murakawa** (University of Toyama)
Numerical simulations of nonlinear cross-diffusion systems using a linear scheme

Coffee & Poster break

Evening session (room 103, chairperson: Shinichi Miura)
16:00-16:40 **Makoto Iima** (Hokkaido University)
Numerical simulation and mathematical analysis of flapping flight problem
16:40-16:55 **Muhamad Koyimatu** (Kanazawa University & Bandung Institute of Technology)
Quantum control of high harmonic generation in anharmonic potential
16:55-17:10 **Athiya M. Hanna** (Kanazawa University & Bandung Institute of Technology)
High-pressure crystal structure prediction using evolutionary algorithm simulation
17:10-17:25 **Nyayu Siti Nurainun** (Kanazawa University & Bandung Institute of Technology)
Hydrogen impurities in graphene: first principles study
17:25-17:40 **Micke Rusmerryani** (Kanazawa University & Bandung Institute of Technology)
Molecular dynamics studies on structure and dynamics of spherical micelles
17:40-17:55 **Gia Septiana Wulandari** (Kanazawa University & Bandung Institute of Technology):
Temperature effects on dynamics of spherical micelles: a molecular dynamics study

February 16 (Wednesday): 2nd day

Morning session (room 103, chairperson: Shinichi Miura)

10:00-10:40 **Hitoshi Imai** (University of Tokushima)
Numerical simulation on non-existence and non-uniqueness of solutions for the Tricomi equation

10:40-11:20 **Sparisoma Viridi** (Bandung Institute of Technology)
Self-siphon simulation using molecular dynamics method: a preliminary study

11:20-12:00 **Zaki Su'ud** (Bandung Institute of Technology)
Unprotected loss of flow simulation in fast reactor safety analysis

Lunch break

Afternoon session 1 (room 103, chairperson: Fumiyuki Ishii)

14:00-14:25 **Hiroaki Saito** (Kanazawa University)
Hydration property of globular proteins: a molecular dynamics study

14:25-14:50 **Kazutomo Kawaguchi** (Kanazawa University)
The molecular dynamics simulation of protein complexes

14:50-15:15 **Tatsuki Oda** (Kanazawa University)
Toward a computer modeling in magnetic anisotropy and its electric-field-control for nano-structures

15:15-15:40 **Shinichi Miura** (Kanazawa University)
Variational path integral molecular dynamics method applied to molecular vibrational fluctuations

Afternoon session 2 (room 104, chairperson: Hideki Murakawa)

14:00-14:40 **Katsuyuki Ishii** (Kobe University)
Mathematical analysis for an approximation scheme to mean curvature flow

14:40-15:20 **Takeshi Fukao** (Kyoto University of Education)
Variational inequality for the Navier-Stokes equations with time dependent constraint

15:20-15:40 **Elliott Ginder** (Kanazawa University)
A variational method for volume-controlled membrane motions

Coffee & Poster break

Evening session 1 (room 103, chairperson: Tatsuki Oda)

16:20-16:50 **Phung Thi Viet Bac** (AIST)
Theoretical investigations of hydrogen diffusion into metallic nanoparticles

16:50-17:15 **Fumiyuki Ishii** (Kanazawa University)
First-principles study of ferroelectricity in hydrogen-bonded molecular systems

17:15-17:40 **Mineo Saito** (Kanazawa University)
First-principles calculations of defects in graphenes

17:40-17:55 **Shuhei Kawamoto** (Kanazawa University)
Free energy of peptide to permeate lipid bilayer membrane -- coarse-grained simulation

17:55-18:10 **Muhammad Ilyas** (Kanazawa University & Bandung Institute of Technology)
Generalized extended Hamming codes over Galois ring of characteristic 2^n

Evening session 2 (room 104, chairperson: Takeshi Fukao)

16:20-17:00 **Naoto Nakano** (Hokkaido University)
On steady simple shear flows of a continuum model with density gradient-dependent stress

17:00-17:25 **Hiroshi Iwasaki** (Kanazawa University)
Numerical simulation of Biot's consolidation problem

17:25-17:40 **Triati Dewi Kencana Wungu** (Osaka University)
Study of lithium montmorillonite by ab initio calculation

February 17 (Thursday): 3rd day

Morning session (room 301, chairperson: Hiroaki Saito)

9:20-9:35 **Putu Harry Gunawan** (Kanazawa University & Bandung Institute of Technology)
Simulation of surface detection and surface tension with smoothed particle hydrodynamics

9:35-9:50 **Mourice C. K. Woran** (Kanazawa University & Bandung Institute of Technology)
Simulation of fluid-solid interaction using moving particle semi-implicit and spring-mass system

9:50-10:05 **Ruddy Kurnia** (Kanazawa University & Bandung Institute of Technology)
A novel scheme smoothed particle hydrodynamics to overcome energy loss

10:05-10:20 **Christian Fredy Naa** (Kanazawa University & Bandung Institute of Technology)
Explicit step improvement on moving particle semi-implicit and its analysis by using surface detection algorithm

Coffee & Poster break

10:50-11:30 **Akhmaloka** (Bandung Institute of Technology)
Thermophilic microorganisms and thermostable enzyme from Indonesia hot springs

11:30-12:00 **Hidemi Nagao** (Kanazawa University)
Reduction potential of blue copper proteins

List of Participants

Akhmaloka	Rector of Bandung Institute of Technology, Indonesia
Phung Thi Viet Bac	Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Japan, E-mail: phung.bac@aist.go.jp
Takeshi Fukao	Department of Mathematics, Faculty of Education, Kyoto University of Education, Japan, E-mail: fukao@kyokyo-u.ac.jp
Elliott Ginder	Graduate School of Natural Science and Technology, Kanazawa University, Japan, E-mail: eginder@polaris.s.kanazawa-u.ac.jp (PhD student)
Putu Harry Gunawan	KU-ITB Double-Degree Program* Master Student, E-mail: erik_mathboy@yahoo.com
Laksana Tri Handoko	Group for Theoretical and Computational Physics Research Center for Physics, Indonesian Institute of Sciences, Indonesia, E-mail: handoko@teori.fisika.lipi.go.id
Athiya Mahmud Hanna	KU-ITB Double-Degree Program* Master Student, E-mail: athiya_mh@yahoo.com
Suprijadi Haryono	Faculty of Mathematics and Natural Sciences, Bandung Institute of Technology, Indonesia, E-mail: supri@fi.itb.ac.id
Yasuaki Hiwatari	Toyota Physical and Chemical Research Institute, Japan
Makoto Iima	Department of Mathematics, Hokkaido University, Japan, E-mail: makoto@nsc.es.hokudai.ac.jp
Muhammad Ilyas	KU-ITB Double-Degree Program* Master Student, E-mail: reiken7@gmail.com
Hitoshi Imai	Department of Applied Physics and Mathematics, Faculty of Engineering, University of Tokushima, Japan, E-mail: imai@pm.tokushima-u.ac.jp
Fumiyuki Ishii	Institute of Science and Engineering, Kanazawa University, Japan, E-mail: fumiyuki@kanazawa-u.ac.jp
Katsuyuki Ishii	Faculty of Maritime Sciences, Kobe University, Japan, E-mail: ishii@maritime.kobe-u.ac.jp
Hiroshi Iwasaki	Institute of Science and Engineering, Kanazawa University, Japan, E-mail: iwasaki@cs.s.kanazawa-u.ac.jp
Kazutomo Kawaguchi	Institute of Science and Engineering, Kanazawa University, Japan, E-mail: kkawa@wriron1.s.kanazawa-u.ac.jp
Shuhei Kawamoto	Graduate School of Natural Science and Technology, Kanazawa University, Japan, E-mail: kawamoto@wriron1.s.kanazawa-u.ac.jp (PhD student)
Masaki Kazama	Fujitsu Limited Next Generation Technical Computing Unit, E-mail: kazama.masaki@jp.fujitsu.com
Muhamad Koyimatu	KU-ITB Double-Degree Program* Master Student, E-mail: koyimatu@wriron1.s.kanazawa-u.ac.jp
Ruddy Kurnia	KU-ITB Double-Degree Program* Master Student, E-mail: ruddy.kurnia@gmail.com
Wicharn Lewkeeratiyutkul	Department of Mathematics, Faculty of Science, Chulalongkorn University, E-mail: Wicharn.L@chula.ac.th

Muhamad Abdulkadir Martoprawiro	Faculty of Mathematics and Natural Sciences, Bandung Institute of Technology, Indonesia, E-mail: muhamad@chem.itb.ac.id
Khamron Mekchay	Department of Mathematics, Faculty of Science, Chulalongkorn University, Email: k.mekchay@gmail.com
Shinichi Miura	Institute of Science and Engineering, Kanazawa University, Japan, E-mail: smiura@mail.kanazawa-u.ac.jp
Hideki Murakawa	Graduate School of Science and Engineering for Research, University of Toyama, Japan, E-mail: murakawa@sci.u-toyama.ac.jp
Christian Fredy Naa	KU-ITB Double-Degree Program* Master Student, E-mail: chris_mail@yahoo.com
Hidemi Nagao	Institute of Science and Engineering, Kanazawa University, Japan, E-mail: nagao@wriron1.s.kanazawa-u.ac.jp
Naoto Nakano	Hokkaido University, Japan, E-mail: nakano.naoto@gmail.com
Kiyoshi Nishikawa	Institute of Science and Engineering, Kanazawa University, Japan, E-mail: kiyoshi@wriron1.s.kanazawa-u.ac.jp
Nyayu Siti Nurainun	KU-ITB Double-Degree Program* Master Student, E-mail: nyayu@cphys.s.kanazawa-u.ac.jp
Tatsuki Oda	Institute of Science and Engineering, Kanazawa University, Japan, E-mail: oda@cphys.s.kanazawa-u.ac.jp
Shinya Okabe	Faculty of Humanities and Social Sciences, Environmental Sciences, Iwate University, Japan, E-mail: okabes@iwate-u.ac.jp
Seiro Omata	Institute of Science and Engineering, Kanazawa University, Japan, E-mail: omata@kenroku.kanazawa-u.ac.jp
Harno Dwi Pranowo	Austrian-Indonesian Center for Computational Chemistry, Chemistry Department, Faculty of Mathematics and Natural Sciences, Universitas Gadjah Mada, Yogyakarta, Indonesia, E-mail: harnodp@ugm.ac.id
Micke Rusmerryani	KU-ITB Double-Degree Program* Master Student, E-mail: micke@wriron1.s.kanazawa-u.ac.jp
Hiroaki Saito	Institute of Science and Engineering, Kanazawa University, Japan, E-mail: saito@wriron1.s.kanazawa-u.ac.jp
Mineo Saito	Institute of Science and Engineering, Kanazawa University, Japan, E-mail: m-saito@cphys.s.kanazawa-u.ac.jp
Zaki Su'ud	Department of Physics, Bandung Institute of Technology, Indonesia, E-mail: szaki@fi.itb.ac.id
Karel Svadlenka	Institute of Science and Engineering, Kanazawa University, Japan, E-mail: kareru@staff.kanazawa-u.ac.jp
Masako Takasu	Tokyo University of Pharmacy and Life Sciences, E-mail: takasu@toyaku.ac.jp,
Sparisoma Viridi	Nuclear Physics and Biophysics Research Division, Faculty of Mathematics and Natural Sciences, Bandung Institute of Technology, Indonesia, E-mail: dudung@fi.itb.ac.id
Mourice Ceisper Kevin Woran	KU-ITB Double-Degree Program* Master Student, E-mail: moris_3gun@polaris.s.kanazawa-u.ac.jp

Gia Septiana Wulandari	KU-ITB Double-Degree Program* Master Student, E-mail: gia@wriron1.s.kanazawa-u.ac.jp
Triati Dewi Kencana Wungu	Department of Precision Science & Technology and Applied Physics, Graduate School of Engineering, Osaka University, Japan, E-mail: triati@dyn.ap.eng.osaka-u.ac.jp
Mieko Yamada	Institute of Science and Engineering, Kanazawa University, Japan, E-mail: myamada@kenroku.kanazawa-u.ac.jp

* This Double-Degree Program is an educational program based on the agreement of cooperation between Kanazawa University and Bandung Institute of Technology. Therefore, the affiliation of students participating in this program is as follows:

Graduate School of Natural Science and Technology, Kanazawa University, Japan &

Faculty of Mathematics and Natural Sciences, Bandung Institute of Technology, Indonesia