

## International Symposium on Computational Science 2015

**Date:** February 17, 2015 – February 18, 2015

**Venue:** Kanazawa University, Kakuma, Kanazawa 920-1192, Japan  
Incubation Laboratory

**Organized by:**

Faculty of Mathematics and Physics,  
Kanazawa University



Faculty of Mathematics and Natural Sciences,  
Bandung Institute of Technology



**Supported by:**

Computational Material Science Initiative (CMSI)



**Home page:** <http://iscs.w3.kanazawa-u.ac.jp/>

**Program:**

Oral sessions: 17<sup>th</sup> 9:30 – 12:30, 18<sup>th</sup> 9:00 – 10:30, 18<sup>th</sup> 15:00 – 16:30

DDP sessions: 17<sup>th</sup> 13:30 – 17:45

Special session: 18<sup>th</sup> 13:30 – 14:45

Poster session: 18<sup>th</sup> 10:30 – 12:00

**Organizing Committee:**

Kanazawa University: F. Ishii, H. Iwasaki, K. Kawaguchi, M. Kimura, S. Miura, H. Nagao (Chair), T. Oda, S. Omata, H. Saito, M. Saito, K. Svadlenka

Bandung Institute of Technology: Acep Purqon, Finny Oktariani, Triati Dewi Kencana Wungu

Chulalongkorn University: Khamron Mekchay

**International Advisory Board:**

E. T. Baskoro (Bandung), M. A. Martoprawiro (Bandung), Suprijadi (Bandung), M. Saito (Kanazawa)

# Symposium Program

February 17 (Tuesday)

## Morning session 1

Chair: Mineo Saito

9:30-10:00

**Hakim L. Malasan** (Bandung Institute of Technology)

*South-East Asia Astronomy Network on High Performance Computing and Data Analysis*

10:00-10:30

**Tatsuki Oda** (Kanazawa University)

*Implementation of first-principles logarithmic mean force dynamics and strategy to the high performance computing*

## Coffee break

## Morning session 2

Chair: Fumiya Ishii

10:50-11:10

**Masashi Iwayama** (Kanazawa University)

*Computation of redox potential of molecules by energy representation method*

11:10-11:30

**Moh Adhib Ulil Absor** (Kanazawa University)

*Persistent spin helix on ZnO (10-10) surface: First-principles study*

11:30-11:50

**Sholihun** (Kanazawa University)

*Density-functional-theory Calculations of the Germanium Multivacancies*

11:50-12:10

**Masao Obata** (Kanazawa University)

*Non-empirical Study on Oxygen Molecular and Crystal Systems Using Van der Waals Density Functional Approach*

12:10-12:30

**Daiki Yoshikawa** (Kanazawa University)

*Structural and electronic properties and electric field variations of magnetic anisotropy in Fe/MgO interface*

## Lunch break

## DDP session 1

13:30-13:45

**Weerasak Dee-Am** (Kanazawa University, CU, Chair: Seiro Omata)

*Simulation of the motion of a droplet on a plane by the discrete Morse flow*

13:45-14:00

**Ullul Azmy** (Kanazawa University, ITB, Chair: Seiro Omata)

*Simulation of a Rising Oil Droplet using an Interface-Fluid Coupling*

- 14:00-14:15      **Herlan Setiadi** (Kanazawa University, ITB, Chair: Seiro Omata)  
*A Particle Based Solver for the Three Dimensional Fluid Flow through an Elastic Porous Medium*
- 14:15-14:30      **Pornchanit Supvilai** (Kanazawa University, CU, Chair: Seiro Omata)  
*Simulation of A Soap Film Catenoid*
- 14:30-14:45      **Reza Fahrul Arifin** (Kanazawa University, ITB, Chair: Seiro Omata)  
*Triple Junction Simulation using the Acceleration Dependent BMO method*

Coffee break

DDP session 2

- 15:00-15:15      **Armanda Ikhsan** (Kanazawa University, ITB, Chair: Masato Kimura)  
*Finite Element Simulation of Crack Propagation- Exact Solution and Phase Field Model*
- 15:15-15:30      **Maharani Ahsani Ummi** (Kanazawa University, ITB, Chair: Masato Kimura)  
*Shape Optimization Approach to an Inverse Free Boundary Problem*
- 15:30-15:45      **Iryanto** (Kanazawa University, ITB, Chair: Karel Svadlenka)  
*Shallow Water - Navier-Stokes Coupling Method in Ocean Wave Simulation*
- 15:45-16:00      **Fuad Yasin** (Kanazawa University, ITB, Chair: Kenichi Kawagoe)  
*Non-vanishing Terms of the Jones Polynomial*
- 16:00-16:15      **Prihardono Ariyanto** (Kanazawa University, ITB, Chair: Kenichi Kawagoe)  
*The 5-Puzzle and 8-Puzzle with the Neighbors Swap Motion*

Coffee break

DDP session 3

- 16:30-16:45      **Muhammad Zaki Almuzakki** (Kanazawa University, ITB, Chair: Katsuyoshi Ohara)  
*Computing general error locator polynomials of 3-error-correcting BCH codes via syndrome varieties using minimal polynomials*
- 16:45-17:00      **Dinan Andiwijayakusuma** (Kanazawa University, ITB, Chair: Mineo Saito)  
*First Principle Study of Hydrogen Impurity in GaN*
- 17:00-17:15      **Muhammad Rifqi Al Fauzan** (Kanazawa University, ITB, Chair: Mineo Saito)  
*Multiferroic BiFeO<sub>3</sub> for Photovoltaics Application : A First Principle Study*

- 17:15-17:30      **Sri Rahayu Natasia** (Kanazawa University, ITB, Chair: Hidemi Nagao)  
*Prediction of Solvation Free Energy of Proteins: Molecular Dynamics Simulation and QSPR Model Approach*
- 17:30-17:45      **Kazuma Tamura** (ITB, Kanazawa University, Chair: Muhamad A. Martoprawiro)  
*Computing reduction potential of Glucose Oxidase enzyme*
- 18:30-              Banquet at University Canteen (“Minami-Fukuri Frepo”)

## February 18 (Wednesday)

### Morning session

Chair: Karel Svadlenka

9:00-9:30

**Petr Pauš<sup>1),2)</sup>, Michal Beneš<sup>1)</sup>, and Jan Kratochvíl<sup>1)</sup>** (Czech Technical University in Prague<sup>1)</sup>, Meiji University<sup>2)</sup>)

*Numerical simulation of dislocation cross-slip in non-symmetric configurations*

9:30-10:00

**Krung Sinapiromsaran** (Chulalongkorn University)

*Simplex improvement without artificial variables*

10:00-10:30

**Muhamad A. Martoprawiro** (Bandung Institute of Technology)

*Computational study of structure and stability of  $[Fe_n(L_1)_p(L_2)_q]^{x+}$  and  $[Fe_n(L_1)_r]^{y+}$  polymeric complexes with  $n = 2, 4,$  and  $6$ ,  $L_1 = 1,2,4\text{-}4H\text{-}1,2,4\text{-}triazole$ ,  $L_2 = 1,2,4\text{-}triazolato$ ,  $p = 4, 8,$  and  $12$ ,  $q = 2, 4,$  and  $6$ ,  $r = 6, 12,$  and  $18$ ,  $x = 2, 4, 6,$  and  $y = 4, 8, 12$*

### Poster session / Business meeting

10:30-12:00

See below for poster session program

12:00

Group Photo

### Lunch break

### Special session

**Universities Introduction for Studying Abroad** Chair: Masato Kimura

This is a special session for Japanese students in Kanazawa University to study abroad. Some universities with which Faculty of Mathematics and Physics, Kanazawa University has (or is planning to have) student exchange programs are introduced. This session is performed in Japanese and English.

13:30-13:40

**Masato Kimura** (Kanazawa University)

*An encouragement of studying abroad*

13:40-13:50

**Muhamad A. Martoprawiro** (Bandung Institute of Technology)

*Introduction of Bandung Institute of Technology (Bandung, Indonesia)*

13:50-14:00

**Krung Sinapiromsaran** (Chulalongkorn University)

*Introduction of Chulalongkorn University (Bangkok, Thailand)*

14:00-14:10

Question time

14:10-14:20

**Koichi Matsumoto** (Kanazawa University)

*Introduction of Kazan Federal University (Kazan, Russia)*

14:20-14:30

**Masato Kimura** (Kanazawa University)

*Introduction of Eindhoven University of Technology (Eindhoven, Netherlands)*

14:30-14:40 **Petr Pauš** (Czech Technical University, Meiji University)  
*Introduction of Czech Technical University (Prague, Czech Republic)*

14:40-14:45 Question time

Coffee break

Afternoon session Chair: Shinichi Miura

15:00-15:30 **Tsutomu Kawatsu** (The University of Tokyo, Yokohama City University)  
*Application of Ab initio Path Integral Molecular Dynamics to Molecular Systems*

15:30-16:00 **Takashi Uneyama** (Kanazawa University)  
*Modelling and Simulations of Polymeric Systems under Static and Dynamic Constraints*

16:00-16:30 **Tomoaki Niiyama** (Kanazawa University)  
*The molecular dynamics study on non-equilibrium critical behaviors in crystalline plasticity*

Poster session (10:30 – 12:00 February 18)

1. **Weerasak Dee-Am** (Kanazawa University, CU)

*Simulation of the motion of a droplet on a plane by the discrete Morse flow*

2. **Ullul Azmy** (Kanazawa University, ITB)

*Simulation of a Rising Oil Droplet using an Interface-Fluid Coupling*

3. **Herlan Setiadi** (Kanazawa University, ITB)

*A Particle Based Solver for the Three Dimensional Fluid Flow through an Elastic Porous Medium*

4. **Pornchanit Supvilai** (Kanazawa University, CU)

*Simulation of A Soap Film Catenoid*

5. **Reza Fahrul Arifin** (Kanazawa University, ITB)

*Triple Junction Simulation using the Acceleration Dependent BMO method*

6. **Armanda Ikhsan** (Kanazawa University, ITB)

*Finite Element Simulation of Crack Propagation- Exact Solution and Phase Field Model*

7. **Maharani Ahsani Ummi** (Kanazawa University, ITB)

*Shape Optimization Approach to an Inverse Free Boundary Problem*

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*Shallow Water - Navier-Stokes Coupling Method in Ocean Wave Simulation*

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*Non-vanishing Terms of the Jones Polynomial*

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*The 5-Puzzle and 8-Puzzle with the Neighbors Swap Motion*

11. **Muhammad Zaki Almuzakki** (Kanazawa University, ITB)

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*First Principle Study of Hydrogen Impurity in GaN*

13. **Muhammad Rifqi Al Fauzan** (Kanazawa University, ITB)

*Multiferroic BiFeO<sub>3</sub> for Photovoltaics Application : A First Principle Study*

14. **Sri Rahayu Natasia** (Kanazawa University, ITB)

*Prediction of Solvation Free Energy of Proteins: Molecular Dynamics Simulation and QSPR Model Approach*

15. **Kazuma Tamura** (ITB, Kanazawa University)

*Computing reduction potential of Glucose Oxidase enzyme*

16. **Takahiro Ito** (Kanazawa University)

*Analysis of numerical oscillation of Crank-Nicolson method for the heat equation*

17. **Takayuki Noda** (Kanazawa University)

*Wave simulation using Navier-Stokes Equation and Shallow Water Equation Models*

18. **Daiki Yoshikawa** (Kanazawa University)

*Structural and electronic properties and electric field variations of magnetic anisotropy in Fe/MgO interface*



## List of participants

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

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