Conference on Computational Physics (CCP2012)

for Physics, Chemistry, Biology, Engineering and related academic fields and industrial applications

October 14 (Sunday)-18 (Thursday), 2012
The Nichii Gakkan Conference Center, Kobe, Japan
(next to the K-computer site)
Organized by C20, IUPAP
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Welcome to CCP2012

You are welcome to CCP2012, held next to the K computer site in Kobe and in the best season of Japan. The Conference on Computational Physics (CCP) is organized annually under the auspices of the Commission 20 of the IUPAP (International Union of Pure and Applied Physics).

This is the first time it is held in Japan. I was asked to be the chairman about two and half years ago and when I accepted the request I decided to make the conference very unique, different from the traditional style of CCP. I was not satisfied when I attended big conferences where the parallel sessions are classified with the name of the research field. We have many chances to attend domestic and international conferences these days. There it is possible to listen to many talks on the same topics and if the topics are very new, such conference is very useful for my research. I wanted, however, to have some conference where I can listen to a variety of topics carried out with the same method.

Computational science is very unique and it is easy to organize a new type of conference with the classification in the horizontal direction of the matrix made of the names of research fields and the name of numerical methods. You may be able to enumerate easily the name of methods, finite difference, Monte Carlo, particle, molecular dynamics and so on. My dissatisfaction is found to have come from the fact that most of conferences focus on research fields and the method that brings to the scientific research is not highlighted so much. I wanted to listen to topics from fundamental physics to industrial science in a systematic way.

In order to realize such conference, a small number of experts is not enough and I asked the help of more than 100 Japanese computer scientists in a variety of fields. We called this group the Japan Advisory Board (JAB). I asked them to recommend the member of the International Advisory Board (IAB). Then, we could start making the list of plenary speakers and invited speakers. It was almost the end of March this year.

CCP2012 is organized also to celebrate the shared use of the K computer and we selected a venue next to the K computer. The shared use is of course open to the public and started on September 28th, one month earlier than previously scheduled. I hope you also enjoy the guided tour to the K computer.

Throughout CCP2012, I hope new collaborations start among scientists in different fields. It would be also my great pleasure if such an inter-disciplinary conference will encourage young scientists (with their fresh energy and skills) to challenge new topics in different fields, especially emerging ones like bio-computing, industrial applications, social sciences and so on.

Finally, allow me to express my sincere thanks to all members of the local organizing committee (LOC). Twenty scientists from three universities and one institute voluntarily worked very hard to prepare CCP2012 as LOC.

The Chairman, CCP2012

Hideaki Takabe (Aki)
Greetings on behalf of the co-organizing academic societies

Shoji Nagamiya
President of AAPPS and ex-President of JPS

It is my great pleasure to be here at the CCP2012 conference to give an opening address.

First I would like to comment that Moore’s law exists in the computer society. Namely, the computing power is increased twice per 1.5 years. If one waits ten years, the computer power is increased by 100 times, and for the 30 years by $10^6$. This is amazing and this trend, which is similar to Livingston’s law in my field of accelerators, is still continuing. The KEI is on this line, I guess, and it provides many useful applications including basic science. Some physics can develop only by such a high-speed computer.

In the field of physics where I am involved, a Nambu theory was published over 50 years ago. The proton mass was generated by a spontaneous symmetry breaking. However, the calculation of the Nambu theory was not possible until very recently, since it requires parallel processors at very high speeds. This is only one example. I would like to say that physics is being developed with computer power enormously, and some filed can be developed only when high-speed computer became available. Namely, Physics and Computer are benefiting each other. I feel, therefore, it very important to have this type of conference here at this time in Japan.

Secondly, in this greeting, since I am from Association of Asia Pacific Physical Societies called, the AAPPS, I would like to say a few words on this organization. First, the AAPPS is the organization for Asian Physical Society, which is similar to EPS. It has held regular conferences during the past 30 years, first in Singapore. Immediately after the 3rd meeting in Hong Kong in 1988 the organization called the AAPPS, the association, was invented by the effort of Professor C. N. Yang and many others. The 12th meeting will be held in Japan in July of the next year.

The Association consists of 17 countries and regions written shown below.

ASEAN Institute of Physics: svirulh@chula.ac.th
Australian Institute of Physics: http://www.aip.org.au/
The Chinese Physical Society: http://www.cps-net.org.cn/
The Physical Society of Hong Kong: http://www.pshk.org.hk/
Indian Physics Association: www.tifr.res.in/~ipa
Indonesian Physical Society: http://hfi.fisika.net/
The Physical Society of Japan: http://wwwsoc.nii.ac.jp/jps/
The Japan Society of Applied Physics: http://www.jsap.or.jp/english/
The Korean Physical Society: http://www.kps.or.kr/home/kor/
Malaysian Institute of Physics: kuru@um.edu.my
Mongolian Physical Society: gantsog@num.edu.mn
Nepal Physical Society: http://www.nps.org.np/
New Zealand Institute of Physics: http://nzip.rsnz.govt.nz/
Physical Society of Philippines: http://www.nip.upd.edu.ph/spp/
Institute of Physics, Singapore: http://www.physics.nus.edu.sg/~phyips
South East Asia Theoretical Physics Association: kkphua@wspc.com.sg
The Physical Society locate din Taipei: http://psroc.phys.ntu.edu.tw/
Thai Institute of Physics: http://www.geocities.com/thai_physics/
Vietnam National Institute of Physics: http://www.iop.vast.ac.vn
Next year at APPC, C. N. Yang, Japanese Nobel laureate, for example, Makoto Kobayashi, and many others join this conference. We receive support not only from AAPPS but also from Japanese Physical Society, Japanese Society of Applied Physics. We also plan to have joint session with European Physical Society, EPS. This is the third meeting between EPS and AAPPS. The conference will be held at Makuhari, close to the Tokyo Airports, both Narita and Haneda. If you are interested in, we always welcome you.

Finally, I would like to comment that the AAPPS donates for this conference the prize for the best young (but not student) poster, similar to the EPS.

Congratulations of this important conference and wish you a great success of the conference. Please also enjoy Japan.
Greetings on behalf of the co-organizing universities

Saburo Aimoto
Vice-President of Osaka University

Good morning, everybody. I am Saburo Aimoto, the trustee and vice–president of Osaka University in charge of basic science.

I would like to extend greetings to all of you here on behalf of co-organizing four Universities of Kobe University, University of Hyogo, Kyoto University, and Osaka University.

It is a great honor for us to welcome you to the Conference on Computational Physics 2012. We would like to express our thanks to all of participants from the heart, especially ones from overseas countries for attending this conference. We also wish to express our sincere thanks to the Commission 20 of the International Union of Pure and Applied Physics, for they decided to hold this conference in Kobe, Japan on the occasion of start of the open use of the K computer. As co-organizers, we are very glad to hear that more than 400 researchers participated from 44 countries.

I am an organic chemist, not a physicist. However, I am often astonished at the rapid and remarkable progress of computational science. Scientists in this field show us deep insight into the truth hidden behind experimental data, and predict the features that we cannot elucidate otherwise. This conference covers a wide variety of topics from different disciplines. It is really fantastic that topics on computational theory, atomic nucleus, prediction of typhoon behavior, laser fusion, chemical reaction, and biological and artificial nanostructures will be discussed in one conference. This suggests that the approach based on computation should be an essential and core driving force for natural science and technology.

I suppose that this must be true for social science, too. Therefore the role of this conference and peoples expectation for the progress of this field must be enormous. In this sense, we have to recall Dr. Noyori’s great effort. I believe that his foresight and leadership have realized the setting of the K computer. Without his strong faith, the construction of the K computer would have ended in an illusion. I hope this conference will send the strong message of the importance of powerful computer infrastructure to the public.

Finally, we wish to earnestly thank to the member of the International Advisory Board and all members of the local organizing committee for the preparations of this conference.

We hope that this conference will be successful and that computational physics will make brilliant progress from now on.

I am a citizen of Kobe. As one of citizens of Kobe, I am very happy if you enjoy your stay in port city Kobe.

Thank you very much for your attention.
Greetings on behalf of the Japanese ministry, MEXT

Takahiro Hayashi
Director, Office for the Promotion of Computing Science

I’d like to say a few words to congratulate the success of CCP2012 conference. I am very pleased to learn that a lot of researchers came together from more than 40 countries and regions, which, I believe, makes this conference truly international. Then, I’d like to express my appreciation to the chair-person, Prof. Takabe of Osaka University and other supporting committee members for their substantial efforts to hold this conference here in Kobe in such a successful way.

The reason why this conference is held here is K computer, that is located at the nearby RIKEN Institute and I know you are invited to the laboratory tours to see K computer during this conference.

As many of you know, K computer has started its full service since last month for academia and industrial uses. Although the first prize of TOP500 was taken over by Sequoia of LLNL, K computer is still the most powerful computer opened to the public and is now ready for production runs to produce innovative new findings which are obtained by only K computer. This is our primary goal and I believe you will find some of those preliminary results at this meeting.

Today, the computational science is becoming a powerful tool for various research areas, and I believe national competitiveness in both academia and industries of the nations depends on the performances of supercomputers they have. In US, Europe, China, Russia, India and other countries as well as in Japan, the computational science is being recognized to be one of the most important strategic technologies for keeping the competitiveness up. And thus, a lot of countries including Japan have been promoting the computational science intensively world wide.

In order to develop such computational sciences, not only hardware developments but also application promotions are important. Such promotion programs, for example, INCITE of US and PRACE of Europe, have been conducted under the governmental supports. Of course, we have also similar one that 50 % of the K computer resources are delivered to in the fields of Life Science, Material, Prediction and Protection of Disaster, Industrial Applications and Astrophysics.

As I mentioned before, the computational science is a powerful tool for various research areas. This means researchers in various areas could interact with each other through the computational science. Therefore, I believe, the computational science has a possibility to be an engine which promotes a fusion among different research areas and then creates a new science. This is another important role of it. In that sense, the role of this conference is very significant.

Finally, I want to emphasize the following. By keeping close collaborations with US, Europe and other countries, we are anxious to continue our activities for making computational science more useful and more productive than ever. As the result, the computational science will become an indispensable tool in daily R&D activities of academia and manufacturing. And, I anticipate IUPAP C20 and CCP will play an important role at the center of it.

K is opened to international researchers through the peer review system. I hope K will play a significant role to promote international collaborations.
I hope all of you’ll have a fruitful time by sharing the latest research knowledge at this conference. And please enjoy your stay here in Kobe and Kobe Beef. Thank you for your attention.
Young Scientist Prize in Computational Physics

During CCP2012, the Young Scientist Prize in Computational Physics for year 2012 was awarded by IUPAP to Professor Roger Melko (Department of Physics & Astronomy, University of Waterloo, Canada) for his innovative and deep achievements in developing quantum Monte Carlo methods for quantum information theory and condensed matter physics.

Message upon receiving the award

I am honoured to receive the 2012 Young Scientist Prize in Computational Physics, and, given the list of previous recipients who came before me, am particularly humbled and grateful to the IUPAP for this recognition. I would like to take the opportunity to thank all of my many collaborators, without whom I could not have performed this research, especially Matthew Hastings who worked patiently with me to develop the first Monte Carlo measurement techniques for Renyi entropies in 2009. With the wide visibility that accompanies such a prestigious award, I hope that younger generations of scientists will be inspired to examine the connections between condensed matter and information theory through computer simulations in the future.

Summary of the talk presented at CCP2012

Title: The Information Age in Simulations of Quantum Matter

Abstract:
Monte Carlo simulations have been ubiquitous in efforts to simulate and characterize properties of materials, matter, and systems, since the advent of computers themselves. In the last several decades, condensed matter physicists have turned simulation technology to the study of a new set of phenomena, loosely called "emergent", present in striking examples such as quasiparticle excitations with fractional charge. Despite this interest, emergence is notoriously difficult to characterize, since it is often not manifested in traditional correlation functions. Motivated by this, a new set of tools was recently developed that allows one to probe emergent phenomena in Monte Carlo simulations through their entanglement entropy - a concept borrowed from quantum information theory. Remarkably, since certain scaling terms in the entanglement entropy appear to be universal, its utility in characterizing phases and phase transitions may be ubiquitous. Thus, Monte Carlo simulations are poised to play a central role in an upcoming paradigm shift where physicists increasingly rely on concepts of information theory to characterize correlations in condensed matter, materials, and systems.
Poster prizes

At the end of the conference three poster prizes offered by EPS (for students), AAPPS, and CCP2012 were assigned to the following participants.

1) Mr. Francesco Calcavecchia (Johannes Gutenberg Universität, Mainz, Germany)(student)

Message upon receiving the award
I want to thank all the organizer of the event, that was very interesting and useful, and gave me the opportunity to visit a wonderful country such as Japan.

Summary of the poster presented at CCP2012

Title: Variational approach to hydrogen’s electronic structure

Abstract:
Hydrogen has a complex and still not well-understood phase diagram, in particular at very high pressures and temperatures. Computational studies of its phase diagram are convenient, since it is extremely difficult and often impossible to experimentally achieve such a high pressure and temperature. Being able to accurately describe the electronic structure is a key ingredient in this investigation.
The variational approach has the big advantage that it permits to control on the quality of the trial wavefunction used to describe the electronic structure, and it is therefore easy to compare different results (the function that gives a lower variational energy is to be favored). The product of the Slater Determinant given by the orbitals found from a mean field approach and a so-called Jastrow correlation function, that takes two-body correlations into account, has shown to give accurate results and to work well for different phases. Nevertheless, we have investigated also a different trial function, called Shadow Wave Function, that potentially gives an even larger flexibility and allows for even more accurate calculations.
2) Dr. Kamal Kumar Choudhary (Shri Vaishnav Institute of Technology and Science, Indore, India)

Message upon receiving the award

CCP2012 has provided a great opportunity and platform to share and discuss the views and ideas in the interdisciplinary fields of computational physics. Awards presented at CCP2012 will definitely motivate the researchers and young scholars to look forward in the field of their interest. I am very much grateful to organizers of CCP2012 to award me the APPS Best Poster Prize.

Summary of the poster presented at CCP2012

Title: Quantitative analysis of thermoelectric properties of crystalline semiconductors embedded with ErAs nanoparticles.

Abstract:
We quantitatively analyzed the thermo electric figure of merit \( ZT = S^2 \sigma T / \kappa \) which can be enhanced by nanostructuring thermoelectric materials. The key reason for increase in \( ZT \) is the reduction of thermal conductivity (\( \kappa \)) and increase in thermoelectric power (\( S \)) by embedding ErAs nanoparticles in \( \text{In}_{0.53}\text{Ga}_{0.47}\text{As} \) crystalline semiconductors. The lattice thermal conductivity and thermoelectric power were studied by incorporating the scattering of phonons with defects, grain boundaries, electrons and phonons in the model Hamiltonian to evaluate the thermoelectric properties. We found that ErAs nanoparticles provide an additional scatterer to phonons, on inserting the nanoparticles in the crystal the phonon scattering with point defects and grain boundaries become more efficient which cause in decrease the thermal conductivity up to half and increase in thermoelectric power up to double of its value of pure crystal. The temperature dependent of thermal conductivity and thermoelectric power are determined by competition among the several operating scattering mechanisms for the heat carriers which depend on concentration of nanoparticles in the crystal. Numerical analysis of thermoelectric properties from the present analysis will help in designing better thermoelectric materials for thermoelectric applications.
3) **Dr. Muhammad Shabbir** (Department of Materials Engineering Science, Graduate School of Engineering Science Osaka University, Japan)

**Message upon receiving the award**

It was a great experience for me to participate in conference of computational chemistry (CCP2012) held in Kobe, Japan. The real exciting parts were the fascinating poster and plenary lecture sessions though which we have shared our knowledge as well as exchanged our ideas with world leading physicists on many cutting edge issues of computational physics. At the end, the best poster award for our poster came as pleasant surprise to me. It is not only a matter of honor for me but also for our Nakano’s group in Osaka University.

**Summary of the poster presented at CCP2012**

Title: *Interplay between Diradical Characters and Third-Order Nonlinear Optical Properties in Fullerene Systems*

Abstract:

In the modern era, nonlinear optical (NLO) and spintronic materials are two types of hi-tech and smart materials that have versatile properties. As a pioneering attempt towards understanding of the interplay between these two properties, we proposed a new structure-property relationship between the diradical character ($\gamma_i$), which is a chemical index of the bond nature, and the third-order NLO polarizability (second hyperpolarizability, $\gamma$) of open-shell singlet systems. We studied the topological dependence of diradical character and second hyperpolarizability ($\gamma$) in fullerenes. We found that the large differences between the geometry and topology of fullerenes have a significant effect on the diradical character of each fullerene as elucidated by their odd electron densities distributions. On the basis of their different diradical character, these fullerenes were categorized into three groups, that is, closed-shell ($\gamma_i=0$), intermediate open-shell (0<$\gamma_i$<1), and almost pure open-shell compounds ($\gamma_i\approx1$). This categorization has been found in accordance with Clar’s sextet rule that has been applied on Schlegel projections of these fullerenes. For example, we found that closed-shell fullerenes include $C_{20}$, $C_{60}$, and $C_{70}$, whereas fullerenes $C_{26}$ and $C_{36}$ and $C_{30}$, $C_{40}$, $C_{42}$, and $C_{48}$ are pure and intermediate open-shell compounds, respectively. Interestingly, the $\gamma_{zzzz}$ enhancement ratios between $C_{30}/C_{36}$ and $C_{40}/C_{60}$ are 4.42 and 11.75, respectively, regardless of the smaller $\pi$-conjugation size in $C_{30}$ and $C_{40}$ than in $C_{36}$ and $C_{60}$. Larger $\gamma_{zzzz}$ values were obtained for other
fullerenes that had intermediate diradical character that is in line to our previous valence configuration interaction (VCI) results for the two-site diradical model. The $\gamma_{zzz}$ density analysis shows that the large positive contributions originate from the large $\gamma_{zzz}$ density distributions on the right- and left-extended edges of the fullerenes, between which significant spin polarizations (related to their intermediate diradical character) appear within the spin-unrestricted DFT level of theory. On the bases of this structure-property relationship, we have further constructed bucky ferrocenes with robust second hyperpolarizabilities that can be switched on and off in their singlet and triplet ground states, respectively.
Conference organization

The Conference on Computational Physics (CCP) is organized annually under the auspices of the Commission 20 of the IUPAP (International Union of Pure and Applied Physics).

Main purpose of CCP2012

This 24th Conference on Computational Physics aims at stimulating interdisciplinary discussion and collaboration by putting together researchers interested in various fields of computational science, with focus on pure and applied Physics, Chemistry, Biology, Engineering, Climate, Weather, Earth Science and so on.

Distinctive features

1. Broad range of topics.
2. Thirteen plenary talks with comprehensive reviews from theoretical physics to industrial application.
3. Half of the parallel session organized on the basis of numerical methods and the other half about special topics deemed of particular importance.
4. Speakers are invited to present: i) a comprehensive overview of their research field, ii) the reasons why the selected numerical methods are useful or necessary for their computation, iii) numerical scheme and results, and iv) future prospects.

CCP2012 is co-organized by:

Osaka University
Kyoto University
Kobe University
University of Hyogo
The Japan Physical Society (JPS)
The Japan Society of Applied Physics (JSAP)

It is also endorsed by:

The Ministry of Education, Culture, Sports, Science & Technology in Japan (MEXT)
The Advanced Institute for Computational Science (AICS)
Association of Asia-Pacific Physical Societies (AAPPSS)
European Physical Society (EPS)
American Physical Society (APS)
The Asahi Shimbun (The Newspaper Co LTD)
The Kobe Shimbun (The Newspaper Co LTD)
It is supported by:

The Institute of Laser Engineering (ILE), Osaka University
The Research Center for Nuclear Physics (RCNP), Osaka University
The Earth Simulator Center (JAMSTEC)
Chinese Physical Society (CPS)

It is financially supported by:

Japan Society for the Promotion of Science (JSPS)
Japan World Exposition 1970 Commemorative Fund (JEC Fund)
Kobe Convention & Visitor Association
Nakauchi Tsutomu Convention Promotion Foundation
Fujitsu
NEC

History of the Conference on Computational Physics

The Conference on Computational Physics was organized for the first time in 1989 in Boston, and since 2003 it takes place every year, rotating between Europe-Africa, North-South America, and Asia-Oceania. The keynote plenary talks are presented by prominent researchers in each of the several sub-fields of computational physics and its applications.

Past and future editions of the Conference on Computational Physics:

2013 – Moscow, Russia
2012 - Kobe, Japan
2011 - Gatlinburg, USA
2010 - Trondheim, Norway
2009 - Kaohsiung, Taiwan
2008 - Ouro Preto, Brazil
2007 - Brussels, Belgium
2006 - Gyeongju, Republic of Korea
2005 - Los Angeles, California, USA
2004 - Genoa, Italy
2003 - Beijing, China
2002 - San Diego, California, USA
2001 - Aachen, Germany
2000 - Brisbane, Australia
1999 - Atlanta, Georgia, USA
1998 - Granada, Spain
1997 - Santa Cruz, USA
1996 - Cracow, Poland
1995 - Pittsburgh, USA
1994 - Lugano, Switzerland
1993 - Albuquerque, USA
1992 - Prague, Czech Republic
1991 - San Jose, USA

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1990 - Amsterdam, the Netherlands
1989 - Boston, USA
CCP2012 Committees

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DingSheng Wang (Institute of Physics, China)
Kunihiko Watanabe (JAMSTEC, Japan)
Wolfgang Wenzel (KIT, Germany)
Philipp Werner (University of Fribourg, Switzerland)
Naoki Yoshida (IPMU, Japan)
Yasunari Zempo (Hosei University, Japan)

Local Organizing Committee:

Chair: Takahito Nakajima (RIKEN, AICS)
Vice-chair: Ryusuke Numata (University of Hyogo)
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Kei Tokita (Osaka University)
Hirofumi Tomita (RIKEN, AICS)
Shugo Yasuda (University of Hyogo)
Seiji Yunoki (RIKEN, AICS)

More than 100 computational scientists experts in fields ranging from pure physics to industrial applications of physics contributed to the completion of the scientific program.
Guidelines for presenters and session chairpersons

We organized parallel sessions on the basis of numerical methods while including very different topics from fundamental physics to industrial applications. In order for the audience to be able to understand the presentations and join the discussion, each presenter (including plenary speakers) is warmly invited to pay attention to the following points:

1. Explain the background and motivation of your research with easy words at first. Avoid using jargon. Assume the audience has knowledge at the level of an undergraduate.

2. Show the basic equations you are going to solve numerically and show them in a form as simple as possible.

3. Explain why you use your specific numerical method and what the unique and challenging points of that numerical scheme are.

4. Describe what the scientific product and result of your simulation is.

5. Explain how to improve the present numerical methods. Then show what original results you expect with such improved or new numerical methods.

The chairperson of each session is asked to stimulate discussion, also by giving ideas on how to help improve the speaker’s computations.

We hope that in this conference you will enjoy interdisciplinary discussion on forefront research and that new collaborations will start through such discussions between scientists in different fields.

Panel discussion

On Thursday 18th between 11:00 and 12:30 we organized a panel discussion on the subject:

"Will computational science be able to provide answers to important problems of human society?"

The panel started with a plenary talk (30 minutes) by a journalist, Ms Atsuko Tsuji of the Asahi Shimbun. The remaining time was left for discussion. Simultaneous English-Japanese translation will be available.
Several booths will complement the conference, advertising scientific projects and other activities.

- **Booth 1.** Predictable life science, healthcare, and drug discovery foundation (by RIKEN)
- **Booth 2.** New materials and energy creation (by Institute for Solid State Physics of the University of Tokyo; Institute for Molecular Science; Institute for Materials Research, Tohoku University)
- **Booth 3.** Projection of global change toward the mitigation of natural disasters (by Japan Agency for Marine-Earth Science and Technology)
- **Booth 4.** Next-generation manufacturing technology (by Institute of Industrial Science, University of Tokyo; Japan Aerospace Exploration Agency; Japan Atomic Energy Agency)
- **Booth 5.** The origin of matter and the universe (by University of Tsukuba, High Energy Accelerator Research Organization, National Astronomical Observatory of Japan)
- **Booth 6.** Fujitsu Company
- **Booth 7.** Center for Planetary Science, Kobe University
- **Booth 8.** Graduate school of Simulation Studies, University of Hyogo
- **Booth 9.** International Office, Osaka University
# Program at a glance

| Time   | Sunday 14 October | Monday 15 October | Tuesday 16 October | Wednesday 17 October | Thursday 18 October |
|--------|-------------------|-------------------|--------------------|----------------------|---------------------|
| 8:00   | Registration      | Registration      | Registration       | Registration          | Registration        |
| 9:00   | Opening ceremonies | Plenary: Zhu       | Plenary: Okuda     | Plenary: Arsuaga      |                     |
| 9:45   | Plenary: Imada    | Plenary: Pietrucci | Plenary: Pourtois  |                      |                     |
| 10:30  | Break             | Break             | Break              | Break                |                     |
| 11:00  | Plenary: Papenbrock | Plenary: Blügel  | Plenary: Jansen    |                      | Panel discussion    |
| 11:45  | Plenary: Takahashi | Plenary: Melko    | Plenary: Krauth    |                      |                     |
| 12:30  | Lunch             | Lunch             | Lunch              | Lunch                |                     |
| 13:50  | Registration (starting at 15:00) and reception (starting at 17:00) | Parallel sessions | Parallel sessions | Parallel sessions | Parallel sessions |
| 16:00  | Poster session    | Poster session    | Poster session     | Poster session       |                     |
| 19:00  | Banquet           |                   |                    |                      |                     |

## Overview of parallel sessions

| Oct. 15 (Mon) | K-computer special | Quantum Monte Carlo methods | Multi-hierarchy methods | Education in computational physics | Finite-difference, finite-volume, finite-element methods | Density Matrix Renormalization Group | Climate and disaster prevention |
|---------------|---------------------|-----------------------------|-------------------------|-----------------------------------|----------------------------------------------------------|-------------------------------------|----------------------------------|
| Oct. 16 (Tue) | K-computer special | Quantum Monte Carlo methods | Large-scale computing   | Molecular dynamics                | Finite-difference, finite-volume, finite-element methods | Density Functional Theory          | Particle methods                 |
| Oct. 17 (Wed) | Monte Carlo methods | Quantum Monte Carlo methods | Large-scale computing   | Molecular dynamics                | Community-driven codes                                    | Visualization                       | Industrial applications           |
| Oct. 18 (Thu) | Monte Carlo methods | Biocomputing                | Multi-hierarchy methods | Molecular dynamics                | Finite-difference, finite-volume, finite-element methods | Density Functional Theory          | Particle methods                 |
# Daily schedules

## Oct. 14 (Sun)
- 15:00-19:00 Registration
- 17:00-19:00 Reception

## Oct. 15 (Mon)
- **8:00-** Registration
- **9:00-9:45** Opening
  - *Masatoshi Imada*, *Quantum Monte Carlo for strongly correlated systems*, University of Tokyo (Japan)
- **10:30-11:00** Break
- **11:00-11:45** *Thomas Papenbrock*, *Computing the atomic nucleus*, University of Tennessee and Oak Ridge National Laboratory (USA)
- **11:45-12:30** *Keiko Takahashi*, *Challenge toward the prediction of typhoon behavior and downpour*, Japan Agency for Marine-Earth Science and Technology (Japan)
- **12:30-13:50** Lunch
- **13:50-16:00** Parallel sessions
  - **K-computer special**
  - **Quantum Monte Carlo methods**
  - **Multi-hierarchy methods**
  - **Education in computational physics**
  - **Finite-difference, finite-volume, finite-element methods**
  - **Density Matrix Renormaliz. Group**
  - **Climate and disaster prevention**
  - **Rooms**
    - K-computer building (AICS), seminar room 1st floor
    - Kobe University, Convention Hall, 2nd floor
    - Nichii Gakkan Conference Center, 3rd floor hall A
    - Nichii Gakkan Conference Center, 2nd floor room 1
    - Nichii Gakkan Conference Center, 3rd floor hall B
    - Nichii Gakkan Conference Center, 2nd floor room 2
    - Nichii Gakkan Conference Center, 2nd floor room 3
- **16:00-17:30** Poster session (with refreshments available)
- **16:00-16:45** Visit to K computer (group A)
- **16:45-17:30** Visit to K computer (group B)

## Schedule of the opening ceremony
**October 15 (9:00-9:45)**

MC: Luca Baiotti

**Welcome address:**

Hideaki Takabe, Chair of CCP2012

**Greeting on behalf of co-organizing academic societies:**

Shoji Nagamiya, President of AAPPS and ex-President of JPS

**Greeting on behalf of the co-organizing four universities:**

Saburo Aimoto, vice-President of Osaka University

**Greeting on behalf of our ministry, MEXT:**

Takahiro Hayashi, Director, Office for the Promotion of Computing Science

**Greeting on behalf of IUPAP,**
Alex Hansen, Chair of Commission 20 (Computational Physics), IUPAP

### Oct. 16 (Tue)

| Time    | Speaker and Title                                                                 | Organization                  |
|---------|----------------------------------------------------------------------------------|--------------------------------|
| 9:00-9:45 | Shao-Ping Zhu, Computer simulations on laser fusion                              | Institute of Applied Physics and Computational Mathematics (China) |
| 9:45-10:30 | Fabio Pietrucci, Molecular dynamics challenges: from chemical reactions to biological and artificial nanostructures | EPF Lausanne (Switzerland) |
| 10:30-10:50 | Break                                                                          |                                |
| 10:50-11:35 | Stefan Blügel, Computing inhomogeneous solids by density functional theory      | Forschungszentrum Jülich (Germany) |
| 11:35-12:25 | IUPAP Young Scientist Award 2012: Roger Melko, The information age in simulations of quantum matter | University of Waterloo (Canada) |
| 12:25-12:45 | Conference photo, in front of the building of K computer                         |                                |
| 12:45-13:50 | Lunch                                                                           |                                |
| 13:50-16:00 | Parallel sessions                                                               |                                |
|          | K-computer special                                                              |                                |
|          | Quantum Monte Carlo methods                                                     |                                |
|          | Large-scale computing                                                           |                                |
|          | Molecular dynamics                                                              |                                |
|          | Finite-difference, finite-volume, finite-element methods                        |                                |
|          | Density Functional Theory                                                       |                                |
|          | Particle methods                                                                |                                |

| Time    | Session Location                                                                 |
|---------|----------------------------------------------------------------------------------|
| 13:50-16:00 | K-computer building (AICS), seminar room 1<sup>st</sup> floor                    |
|          | Kobe University, Convention Hall 2<sup>nd</sup> floor                            |
|          | Nichii Gakkan Conference Center, 3<sup>rd</sup> floor hall A                     |
|          | Nichii Gakkan Conference Center, 2<sup>nd</sup> floor room 1                      |
|          | Nichii Gakkan Conference Center, 3<sup>rd</sup> floor hall B                      |
|          | Nichii Gakkan Conference Center, 2<sup>nd</sup> floor room 2                      |
|          | Nichii Gakkan Conference Center, 2<sup>nd</sup> floor room 3                      |
| 16:00-17:30 | Poster session (with refreshments available)                                     |

### Oct. 17 (Wed)

| Time    | Speaker and Title                                                                 | Organization                  |
|---------|----------------------------------------------------------------------------------|--------------------------------|
| 9:00-9:45 | Motoi Okuda, Development of K-computer and toward exascale computing             | Fujitsu (Japan)               |
| 9:45-10:30 | Geoffrey Pourtois, Modeling challenges in nanoelectronics: an atomistic point of view | Imec (Belgium)                |
| 10:30-11:00 | Break                                                                          |                                |
| 11:00-11:45 | Karl Jansen, Lattice computations for high energy and nuclear physics          | DESY (Germany)                |
| 11:45-12:30 | Werner Krauth, Hard-disk melting: New algorithms, new insights                  | École Normale Supérieure (France) |
| 12:30-13:50 | Lunch                                                                           |                                |
| 13:50-16:00 | Parallel sessions                                                               |                                |
|          | Industrial applications                                                          |                                |
|          | Visualization                                                                   |                                |
|          | Large-scale computing                                                           |                                |
|          | Molecular dynamics                                                              |                                |
|          | Quantum Monte Carlo methods                                                     |                                |
|          | Community-driven codes                                                          |                                |
|          | Monte Carlo methods                                                             |                                |

| Time    | Session Location                                                                 |
|---------|----------------------------------------------------------------------------------|
| 13:50-16:00 | K-computer building (AICS), seminar room 1<sup>st</sup> floor                    |
|          | Kobe University, Convention Hall 2<sup>nd</sup> floor                            |
|          | Nichii Gakkan Conference Center, 3<sup>rd</sup> floor hall A                     |
|          | Nichii Gakkan Conference Center, 2<sup>nd</sup> floor room 1                      |
|          | Nichii Gakkan Conference Center, 3<sup>rd</sup> floor hall B                      |
|          | Nichii Gakkan Conference Center, 2<sup>nd</sup> floor room 2                      |
|          | Nichii Gakkan Conference Center, 2<sup>nd</sup> floor room 3                      |
| 16:00-17:30 | Poster session (with refreshments available)                                     |
Oct. 18 (Thu)

9:00-9:45  F. Javier Arsuaga, *Modeling topological changes of highly confined DNA: Applications to the genomic organization of bacteriophages and trypanosomes*, San Francisco State University (USA)

9:45-10:30 Luciano Rezzolla, *Using numerical relativity to explore fundamental physics and astrophysics*, Albert Einstein Institute (Germany)

10:30-11:00 Break

11:00-12:30 Panel discussion: *Will computational science be able to provide answers to important problems of human society?*

12:30-13:50 Lunch

13:50-16:00 Parallel sessions

| Rooms          | Biocomputing | Monte Carlo methods | Multi-hierarchy methods | Molecular dynamics | Finite-difference, finite-volume, finite-element methods | Density Functional Theory | Particle methods |
|----------------|--------------|---------------------|-------------------------|------------------|---------------------------------------------------------|--------------------------|-----------------|
| K-computer building (AICS), seminar room 1st floor | Kobe University, Convention Hall, 2nd floor | Nichii Gakkan Conference Center, 3rd floor hall A | Nichii Gakkan Conference Center, 2nd floor room 1 | Nichii Gakkan Conference Center, 3rd floor hall B | Nichii Gakkan Conference Center, 2nd floor room 2 | Nichii Gakkan Conference Center, 2nd floor room 3 |

16:00-16:20 Break

16:20-16:50 Poster awards and closing

17:00-17:45 Visit to K computer (group E)

Parallel Sessions

**October 15th (Monday)**

**Finite-difference, finite-volume, finite-element methods (October 15th)**

| Location: Nichii Gakkan Conference Center, 3rd floor, hall B | Chairperson: Brian Van Straalen |
|-------------------------------------------------------------|---------------------------------|
| 13:50-14:20  Hideo Aochi, *Finite difference simulations of seismic wave propagation for understanding earthquake physics and predicting ground motions: Advances and challenges*, Bureau de Recherches Géologiques et Minières (France) |
| 14:20-14:50  Petar Mimica, *Numerical simulations of dynamics and emission from relativistic astrophysical jets*, Universidad de Valencia (Spain) |
| 14:50-15:10  CANCELLED |
| 15:10-15:30  Takayuki Umeda, *Global Vlasov simulation on magnetospheres of astronomical objects*, Nagoya University (Japan) |
| 15:30-15:50  Jerome Breil, *Multi-material reconnection-based arbitrary Lagrangian Eulerian (ReALE) method*, CELIA (France) |
### Quantum Monte Carlo methods (October 15th)

| Time         | Speaker                  | Title                                                                                           | Institution                                |
|--------------|--------------------------|-------------------------------------------------------------------------------------------------|---------------------------------------------|
| 13:50-14:20  | CANCELLED                |                                                   |                                             |
| 14:20-14:50  | Michele Casula           | Variational Monte Carlo approaches as a route to describe strongly correlated materials from a fully ab-initio perspective | Pierre and Marie Curie University (France)  |
| 14:50-15:20  | Ting-Wai Chiu            | Simulation of lattice QCD with domain-wall fermions                                             | National Taiwan University (Taiwan)         |
| 15:20-15:40  | Nils Blümer              | Momentum-dependent pseudogaps in the half-filled two-dimensional Hubbard model                   | Johannes Gutenberg University (Germany)     |
| 15:40-16:00  | Satoshi Morita           | Many-variable variational Monte Carlo calculations of the J_1-J_2 Heisenberg model               | University of Tokyo (Japan)                |

### Density Matrix Renormalization Group (October 15th)

(including Direct Matrix Diagonalization, Matrix product states, PEPS, MERA ...)

| Time         | Speaker                  | Title                                                                                           | Institution                                |
|--------------|--------------------------|-------------------------------------------------------------------------------------------------|---------------------------------------------|
| 13:50-14:20  | Pieter Maris             | No Core CI calculations for light nuclei with chiral 2- and 3-body forces                         | Iowa State University (USA)                 |
| 14:20-14:50  | Valentin Zauner          | Calculating excited states of 1D lattice systems with Matrix Product States                      | University of Vienna (Austria)              |
| 14:50-15:10  | Kenji Harada             | Numerical study of incommensurability of the spiral state on spin-1/2 spatially anisotropic triangular antiferromagnets using entanglement renormalization | Kyoto University (Japan)                    |
| 15:10-15:30  | Nicolas Lucien Jean      | Computational issues of configuration interaction frameworks describing open quantum systems     | University of Tennessee (USA)               |
| 15:30-15:50  | Takashi Abe              | Recent development of Monte Carlo shell model and its application to no-core calculations        | University of Tokyo (Japan)                |

### Multi-hierarchy methods (October 15th)

| Time         | Speaker                  | Title                                                                                           | Institution                                |
|--------------|--------------------------|-------------------------------------------------------------------------------------------------|---------------------------------------------|
| 13:50-14:20  | Alphonse Finel           | Inertia dominated criticality in martensites                                                   | Laboratoire d’Etudes des Microstructures, ONERA-CNRS (France) |
| 14:20-14:50  | Ryoichi Yamamoto         | Multiscale simulations of polymeric flow                                                        | Kyoto University (Japan)                    |
| 14:50-15:20  | Valentina Vetere         | From ab-initio to multiscale modeling of electrochemical systems                               | CEA/LITEN (France)                          |
| 15:20-15:40  | Nina Elkina              | Adaptive mesh refinement method for computational electromagnetics and plasma physics         | Ludwig-Maximilians University of Munich (Germany) |
| 15:40-16:00  | CANCELLED                |                                                   |                                             |
### Climate and disaster prevention (October 15th)

**Location:** Nichii Gakkan Conference Center, 2nd floor, room 3  
**Chairperson:** Keiko Takahashi

| Time       | Speaker                  | Title                                                                                     | Institution                                                                 |
|------------|--------------------------|-------------------------------------------------------------------------------------------|------------------------------------------------------------------------------|
| 13:50-14:20| Yoshiyuki Kaneda         | Advanced simulation research on earthquake and tsunami for disaster mitigation,           | Japan Agency for Marine-Earth Science and Technology (Japan)                  |
| 14:20-14:50| Aysen Ergin              | Computational challenges of coasts: Disaster prevention and adaptation                    | Middle East Technical University (Turkey)                                     |
| 14:50-15:20| Muneo Hori               | Earthquake response simulation of structures and urban areas using HPC                   | University of Tokyo (Japan)                                                  |
| 15:20-15:50| Masaki Satoh             | The global cloud-resolving simulation by the Nonhydrostatic Icosahedral Atmospheric Model, NICAM | University of Tokyo (Japan)                                                  |
| 15:50-16:20| Phil Cummins             | New Bayesian approaches to geophysical data inference on parallel computers               | Australian National University (Australia)                                   |
| 16:20-16:40| Takane Hori              | Numerical experiment of sequential data assimilation for crustal deformation between Tonankai and Nankai earthquakes | Japan Agency for Marine-Earth Science and Technology (Japan)                  |

### Education in computational physics (October 15th)

**Location:** Nichii Gakkan Conference Center, 2nd floor, room 1  
**Chairperson:** Joan Adler

| Time       | Speaker                  | Title                                                                                     | Institution                                                                 |
|------------|--------------------------|-------------------------------------------------------------------------------------------|------------------------------------------------------------------------------|
| 13:50-14:20| Nithaya Chetty           | Probing the extensive nature of entropy                                                   | University of Pretoria (South Africa)                                        |
| 14:20-14:50| Steven Gottlieb          | From many students per VAX to many cores per student: Some thoughts on teaching computational physics | Indiana University (USA)                                                    |
| 14:50-15:20| Knut Mørken              | Integrating computational methods throughout the bachelor education                        | Oslo University (Norway)                                                    |
| 15:20-15:40| Kihyeon Cho              | The fusion research of theory-experiment-simulation for particle physics                  | Korean Institute of Science and Technology Information (Republic of Korea)    |

### K-computer special (October 15th)

**Location:** K-computer building (AICS), seminar room, 1st floor  
**Chairperson:** Atsushi Oshiyama

| Time       | Speaker                  | Title                                                                                     | Institution                                                                 |
|------------|--------------------------|-------------------------------------------------------------------------------------------|------------------------------------------------------------------------------|
| 13:50-14:20| Shinobu Yoshimura        | Petascale simulations of nuclear power plants subjected to strong earthquakes on K-computer | University Tokyo (Japan)                                                    |
| 14:20-14:50| Kazuo Kitaura            | Large scale quantum chemical calculations on biomolecules                                 | Kobe University (Japan)                                                      |
| 14:50-15:20| Hideaki Fujitani         | High performance computing for drug development on K computer                              | University of Tokyo (Japan)                                                 |
| 15:20-15:50| Takaharu Otsuka          | New horizon of computational nuclear structure physics in the K-computer era               | University of Tokyo (Japan)                                                 |
### October 16th (Tuesday)

#### Finite-difference, finite-volume, finite-element methods (October 16th)

| Time      | Speaker                  | Title                                                                 | Institution                                           |
|-----------|--------------------------|----------------------------------------------------------------------|-------------------------------------------------------|
| 13:50-14:20 | Kozo Fujii               | Spectral-like schemes and their application to CFD study toward innovation | Japan Aerospace Exploration Agency (JAXA) (Japan)     |
| 14:20-14:50 | Maxime Viallet           | Time-accurate implicit methods for the modeling of low to moderate Mach number flows in stellar interiors | University of Exeter (UK)                            |
| 14:50-15:10 | Pedro Montero           | BSSN equations in spherical coordinates without regularization: vacuum and non-vacuum spherically symmetric spacetimes | Max Planck Institute for Astrophysics (Germany)       |
| 15:10-15:30 | CANCELLED                |                                                                      |                                                       |
| 15:30-15:50 | Ming-Yi Lee             | Three-Dimensional Finite Element Simulation of Reflectance of Sub-Wavelength Structures on Silicon Nitride for Solar Cells | National Chiao Tung University (Taiwan)                |

#### Particle methods (October 16th)

| Time      | Speaker                  | Title                                                                 | Institution                                           |
|-----------|--------------------------|----------------------------------------------------------------------|-------------------------------------------------------|
| 13:50-14:20 | Luís O. Silva           | Modeling of multiscale extreme plasma physics scenarios with the Osiris particle-in-cell framework | Instituto Superior Técnico, Lisbon (Portugal)         |
| 14:20-14:50 | Kohji Yoshikawa         | An alternative to N-body methods in astrophysical self-gravitating systems: Vlasov-Poisson simulations | University of Tsukuba (Japan)                         |
| 14:50-15:10 | Nils Moschüring         | Divergence-free particle merging using energy conserving particle pushing | Ludwig-Maximilians University of Munich (Germany)    |
| 15:10-15:30 | Sebastiano Fabio Schifano | Exploiting parallelism in many-core architectures: a test case based on Lattice Boltzmann Models | University of Ferrara and INFN (Italy)                |
| 15:30-15:50 | Mingyu Zhang            | An improved surface tension model for numerical simulation of interfacial flow by Smoothed Particle Hydrodynamics method | Institute of Applied Physics and Computational Mathematics (China) |
## Molecular Dynamics (October 16th)

| Time          | Speaker                          | Title                                                                 | Institution                                |
|---------------|----------------------------------|----------------------------------------------------------------------|--------------------------------------------|
| 13:50-14:20   | Ryoji Asahi                     | *Extension of applicability of molecular dynamics in Li ion battery* | Toyota Central R&D Lab. (Japan)           |
| 14:20-14:50   | Roland Faller                   | *Molecular modeling as a tool for nano-biotechnology*                | University of California at Davis (USA)   |
| 14:50-15:20   | Timothy C. Germann              | *Molecular dynamics studies of material dynamics: from petascale to exascale* | Los Alamos National Lab (USA)             |
| 15:20-15:40   | Titus Adrian Beu                | *Nanofluidic Transport and field-effect conductance in voltage-controlled carbon nanotubes* | University Babes-Bolyai, Cluj-Napoca (Romania) |
| 15:40-16:00   | Tomás Miguel Sintes             | *Optimal ring size in magnetic filaments*                           | Institute for Cross-disciplinary Physics and Complex Systems (Spain) |

## Quantum Monte Carlo methods (October 16th)

| Time          | Speaker                          | Title                                                                 | Institution                                |
|---------------|----------------------------------|----------------------------------------------------------------------|--------------------------------------------|
| 13:50-14:20   | Shinji Ejiri                     | *Numerical study of QCD phase structure at finite temperature and density* | Niigata University (Japan)                 |
| 14:20-14:50   | Stefano Gandolfi                 | *Neutron matter equation of state, symmetry energy and neutron stars* | Los Alamos National Lab (USA)              |
| 14:50-15:10   | Americo Tristao Bernardes       | *Unveiling global innovation networks*                               | Universidade Federal de Ouro Preto (Brazil) |
| 15:10-15:30   | Tooru Yoshida                    | *Cluster structure obtained from Monte Carlo shell model calculation* | University of Tokyo (Japan)               |
| 15:30-15:50   | Shixun Zhang                     | *A study of parallelizing O(N) Green-Function-Based Monte Carlo method for many fermions coupled with classical degrees of freedoms* | University of Tsukuba (Japan)              |

## Density Functional Theory (October 16th)

| Time          | Speaker                          | Title                                                                 | Institution                                |
|---------------|----------------------------------|----------------------------------------------------------------------|--------------------------------------------|
| 13:50-14:20   | Silke Biermann                   | *First principles calculations for correlated electron materials -- where do we stand?* | École Polytechnique, Palaiseau (France)    |
| 14:20-14:50   |                                 | CANCELLED                                                             |                                            |
| 14:50-15:20   | Minoru Otani                    | *Computer simulations on electrode-electrolyte interface in batteries* | National Institute of Advanced Industrial Science and Technology (Japan) |
| 15:20-15:40   | Van An Dinh                     | *Can a small polaron form in Olivine LiNiPO4? A Hybrid functional study on the polaron-vacancy complex diffusion* | National Institute for Materials Science (Japan) |
| 15:40-16:00   | Yoong-Kee Choe                   | *Nature of proton transport in polymer electrolyte membranes for fuel cell applications: A first-principles molecular dynamics study* | National Institute of Advanced Industrial Science & Technology (Japan) |
### Large-scale computing (present and future prospects) (October 16th)

| Time       | Speaker                          | Title                                                                 | Institution                                      |
|------------|----------------------------------|----------------------------------------------------------------------|--------------------------------------------------|
| 13:50-14:20| Michael Norman                  | Large scale simulations of cosmic reionization,                      | San Diego Supercomputer Center (USA)             |
| 14:20-14:50| Emanuel Gull                    | Large cluster dynamical mean field simulations for Hubbard models,    | University of Michigan (USA)                     |
| 14:50-15:10| CANCELLED                       |                                                                      |                                                  |
| 15:10-15:30| Truong Vinh Truong Duy         | A three-dimensional domain decomposition method for large-scale ab initio electronic structure calculations, | Japan Advanced Institute of Science and Technology (Japan) |

### K-computer special (October 16th)

| Time       | Speaker                          | Title                                                                 | Institution                                      |
|------------|----------------------------------|----------------------------------------------------------------------|--------------------------------------------------|
| 13:50-14:20| Kazuo Saito                     | Super high-resolution mesoscale weather prediction                   | Meteorological Research Institute (Japan)        |
| 14:20-14:50| Atsushi Oshiyama                 | Real-Space-Density-Functional approach to electronic properties of nanostructures, | University of Tokyo (Japan)                      |
| 14:50-15:20| Norbert Attig                   | JUQUEEN: A multi-petaflop IBM Blue Gene/Q system at Jülich for science and engineering in Europe, | Forschungszentrum Jülich (Germany)               |
| 15:20-15:40| Tomoaki Ishiyama                | Petascale cosmological N-body simulations on K Computer,            | Tsukuba University (Japan)                       |

### October 17th (Wednesday)

### Molecular Dynamics (October 17th)

| Time       | Speaker                          | Title                                                                 | Institution                                      |
|------------|----------------------------------|----------------------------------------------------------------------|--------------------------------------------------|
| 13:50-14:20| Stéphane Mazevet                | Simulating matter under extreme conditions,                        | Laboratoire Univers et Théories (LUTH) (France)  |
| 14:20-14:50| Ivana Savic                     | Molecular dynamics and Monte Carlo approaches to thermal transport in nanostructured materials, | University of California at Davis (USA)         |
| 14:50-15:20| Enge Wang                       | Surface studies of ice,                                             | Peking University (China)                        |
| 15:20-15:40| Vladimir Stegailov             | Atomistic simulation of ultrafast laser ablation of gold: Effect of electronic pressure relaxation, | Joint Institute for High Temperatures, Russian Academy of Sciences (Russian Federation) |
| 15:40-16:00| Hongsuk Yi                     | Parallel programming in Intel MIC architecture,                     |                                                  |
## Monte Carlo methods (October 17th)

**Location:** Nichii Gakkan Conference Center, 2nd floor, room 3  
**Chairperson:** Lev N. Shchur

| Time       | Speaker                          | Title                                                                                           | Institution                                      |
|------------|----------------------------------|-------------------------------------------------------------------------------------------------|--------------------------------------------------|
| 13:50-14:10 | Tor Nordam                       | *The validity of the reduced Rayleigh equation*                                                   | Norwegian University of Science and Technology (Norway) |
| 14:10-14:30 | Sakineh Hosseinabadi             | *Stochastic and fractal properties of silicon and porous silicon rough surfaces*                 | Islamic Azad University, East Tehran Branch (Iran) |
| 14:30-14:50 | Ingve Simonsen                   | *Photonics on the computer*                                                                     | Norwegian University of Science and Technology (Norway) |
| 14:50-15:10 | Andreas Tröster                  | *Optimized Fourier Monte Carlo simulation of crystalline membranes*                              | Vienna University of Technology (Austria)         |
| 15:10-15:30 | Sally J. Bridgewater             | *Adapting phase-switch Monte Carlo for use with flexible organic molecules*                     | University of Warwick (UK)                       |
| 15:30-15:50 |                                | CANCELLED                                                                                       |                                                   |

## Quantum Monte Carlo methods (October 17th)

**Location:** Nichii Gakkan Conference Center, 3rd floor, hall B  
**Chairperson:** Karl Jansen

| Time       | Speaker                          | Title                                                                                           | Institution                                      |
|------------|----------------------------------|-------------------------------------------------------------------------------------------------|--------------------------------------------------|
| 13:50-14:20 | Manolo Per                       | *Calculating physical properties with electronic-structure quantum Monte Carlo*                 | Commonwealth Scientific and Industrial Research Organisation (Australia) |
| 14:20-14:50 | Naoki Kawashima                  | *Quantum Monte Carlo simulations of deconfined critical point*                                  | Institute for Solid State Physics (Japan)         |
| 14:50-15:10 | Denis Perret-Gallix              | *Computational particle physics for event generators and data analysis*                         | IN2P3/CNRS (France)                              |

## Industrial applications (October 17th)

**Location:** K-computer building (AICS), seminar room, 1st floor  
**Chairperson:** Yasunari Zempo

| Time       | Speaker                          | Title                                                                                           | Institution                                      |
|------------|----------------------------------|-------------------------------------------------------------------------------------------------|--------------------------------------------------|
| 13:50-14:20 | Chisachi Kato                    | *Industrial applications of large-scale fluid-dynamics simulations*                              | University of Tokyo (Japan)                      |
| 14:20-14:50 | Erich Wimmer                     | *Computational materials science and engineering: achievements, challenges, and perspectives*    | Materials Design, Inc. (USA and France)           |
| 14:50-15:20 | Masaya Ishida                    | *Computational materials science in industry: Practical applications*                            | Sumitomo Chemical (Japan)                        |
| 15:20-15:50 | Akira Yamaguchi                  | *Simulation based approach in nuclear safety assessment*                                         | Osaka University (Japan)                         |
| 15:50-16:10 | Umar Fauzi                       | *Pore space characterization and fluid flow properties estimation of digital porous materials*    | Institut Teknologi Bandung (Indonesia)            |
### Visualization (October 17th)

| Time    | Speaker                          | Title                                                                                     | Institution                                      |
|---------|----------------------------------|-------------------------------------------------------------------------------------------|--------------------------------------------------|
| 13:50-14:20 | Chandrajit Bajaj             | Enhancing visualization of multiscale biophysical simulations                               | University of Texas at Austin (USA)               |
| 14:20-14:50 | Sam Yang                  | Integrate model and data to visualize microstructures of materials non-destructively       | Commonwealth Scientific and Industrial Research Organisation (Australia) |
| 14:50-15:20 | Akira Kageyama            | Scientific visualization by immersive virtual reality                                      | Kobe University (Japan)                          |
| 15:20-15:40 | Joan Adler                | 3d visualization of atomistic simulations on every desktop                                  | Technion (Israel)                                |
| 15:40-16:00 | Xiao Li                  | Parallel visual analysis for multi-physics petascale simulations                           | Institute of Applied Physics and Computational Mathematics (China) |

### Community-driven codes (October 17th)

| Time    | Speaker                          | Title                                                                                     | Institution                                      |
|---------|----------------------------------|-------------------------------------------------------------------------------------------|--------------------------------------------------|
| 13:50-14:20 | Brian Van Straalen         | Chombo: Still mostly a Cathedral                                                           | Berkeley University (USA)                        |
| 14:20-14:50 | Synge Todo              | The ALPS project: Open source software for strongly correlated systems                    | University of Tokyo (Japan)                      |
| 14:50-15:20 | Frank Löffler            | The Einstein Toolkit: A community code for computational relativistic astrophysics      | Lousiana State University (USA)                  |

### Large-scale computing (present and future prospects) (October 17th)

| Time    | Speaker                          | Title                                                                                     | Institution                                      |
|---------|----------------------------------|-------------------------------------------------------------------------------------------|--------------------------------------------------|
| 13:50-14:20 | Michael Marty Marinak       | New frontiers in the simulation of inertial confinement fusion targets                    | Lawrence Livermore National Laboratory (USA)     |
| 14:20-14:50 | Pablo Ordejón            | Beating the size limits of first-principles calculations in nanoscale systems           | Centre d'Investigació en Nanociència i Nanotecnologia (Spain) |
| 14:50-15:10 | Adam Padee              | Double-layer evolutionary algorithm for distributed optimization of particle detection on the Grid | National Centre for Nuclear Research (Poland)    |
| 15:10-15:30 | Cancelled                 |                                                                                          |                                                  |
## Finite-difference, finite-volume, finite-element methods (October 18th)

| Time       | Speaker                | Title                                                                 | Institution/Location                  |
|------------|------------------------|-----------------------------------------------------------------------|----------------------------------------|
| 13:50-14:20| Yasuhiro Idomura       | Computational challenges in petascale fusion plasma simulations        | Japan Atomic Energy Agency (JAEA) Japan|
| 14:20-14:50| Scott Noble            | Frontiers in computational relativistic magnetohydrodynamics applied to astrophysical systems | Rochester Institute of Technology (USA) |
| 14:50-15:20| Bart van der Holst     | Radiation-hydrodynamic simulations of high-energy-density experiments | University of Michigan (USA)           |
| 15:20-15:40| Yuichiro Sekiguchi     | General relativistic neutrino-radiation (magneto-) hydrodynamics simulations: Formulations and applications | Yukawa Institute for Theoretical Physics (Japan) |
| 15:40-16:00| Ian Hawke              | Numerical simulations of neutron star crusts                           | University of Southampton (UK)         |

## Particle methods (October 18th)

| Time       | Speaker                | Title                                                                 | Institution/Location                  |
|------------|------------------------|-----------------------------------------------------------------------|----------------------------------------|
| 13:50-14:20| Anatoly Spitkovsky     | Kinetic simulations of astrophysical shock waves                       | Princeton University (USA)             |
| 14:20-14:50| Rainer Spurzem        | Astrophysical supercomputing with programmable hardware in China and Germany, Observatories of China, Chinese Academy of Sciences (China) | Heidelberg University (Germany) & National Astronomical Observatories of China, Chinese Academy of Sciences (China) |
| 14:50-15:10| Yosuke Matsumoto      | Electron accelerations at high Mach number shocks: Two-dimensional Particle-in-Cell simulations on massively parallel supercomputer systems | Chiba University (Japan)               |
| 15:10-15:30| CANCELLED              |                                                                       |                                        |
| 15:30-15:50| Go Ogiya              | Study of the core-cusp problem in cold dark matter halos using N-body simulations on GPU clusters | University of Tsukuba (Japan)          |
### Molecular Dynamics (October 18th)

| Time       | Speaker                  | Title and Affiliation                                                                 |
|------------|--------------------------|---------------------------------------------------------------------------------------|
| 13:50-14:20| Richard More            | Molecular dynamics with atomic transitions and nuclear reactions, Lawrence Berkeley National Laboratory (USA) |
| 14:20-14:40| Shinichi Miura          | Development of variational path integral molecular dynamics method with applications to molecular systems, Kanazawa University (Japan) |
| 14:40-15:00| Kim Hyeon-Deuk          | Photoexcited electron and hole dynamics in semiconductor quantum dots: phonon-induced relaxation, multiple exciton generation and recombination, Kyoto University (Japan) |
| 15:00-15:20| Hideo Kaburaki          | A molecular dynamics simulation of fracture process of metals, Japan Atomic Energy Agency (Japan) |
| 15:20-15:40| Shoji Ishibashi        | Computational study of magnetic structure of electron-doped CaMnO3, National Institute of Advanced Industrial Science and Technology (Japan) |
| 15:40-16:00| Satoshi Ohmura          | Dissociation mechanism of bromo aromatic molecules: an ab initio molecular-dynamics study, Kyoto University (Japan) |

### Monte Carlo methods (October 18th)

| Time       | Speaker                  | Title and Affiliation                                                                 |
|------------|--------------------------|---------------------------------------------------------------------------------------|
| 13:50-14:20| Markus Eisenbach        | Thermodynamics of magnetic systems from first principles: Combining Monte-Carlo and Density Functional calculations, Oak Ridge National Lab (USA) |
| 14:20-14:50|                         | CANCELLED                                                                              |
| 14:50-15:10| Lev N. Shchur           | Parallel uncorrelated streams of pseudorandom numbers: problems and solutions, Landau Institute for Theoretical Physics (Russian Federation) |
| 15:10-15:30| Yoshiaki Kato           | Modeling of hot accretion flows around the galactic center black hole, National Astronomical Observatory of Japan (Japan) |
| 15:30-15:50| Paulo Martins           | Probability distribution of the order parameter in the directed percolation universality class, Universidade Federal de Mato Grosso, Brazil (Brazil) |
### Density Functional Theory (October 18th)

| Time     | Speaker               | Title                                                                                   | Institution                                                                 |
|----------|-----------------------|-----------------------------------------------------------------------------------------|------------------------------------------------------------------------------|
| 13:50-14:20 | Thomas Pruschke      | *Reduced Density Matrix Functional Theory - A novel path to treat correlations from first principles?* | Georg-August-Universität Göttingen (Germany)                                 |
| 14:20-14:50 | Jaejun Yu             | *First-principles investigations of strain-dependent magnetism and topological characteristics of quantum materials* | Seoul National University (Republic of Korea)                                |
| 14:50-15:10 | Nguyen Tien Cuong   | *Numerical study on electronic and phononic properties of patterned nano pores structured graphene* | Japan Advanced Institute of Science and Technology (Japan)                     |
| 15:10-15:30 | Shuichiro Ebata      | *Simulation of heavy ion collision using a time-dependent density functional theory including nuclear superfluidity* | University of Tokyo (Japan)                                                  |
| 15:30-15:50 | Manoharan Muruganathan | *Impact of point defects in the graphene nanoribbon on its transport characteristics* | Japan Advanced Institute of Science and Technology (Japan)                     |

### Multi-hierarchy methods (October 18th)

| Time     | Speaker               | Title                                                                                   | Institution                                                                 |
|----------|-----------------------|-----------------------------------------------------------------------------------------|------------------------------------------------------------------------------|
| 13:50-14:20 | Ritoku Horiuchi      | *Multiscale simulations of magnetic reconnection*                                         | National Institute for Fusion Science (NIFS) (Japan)                           |
| 14:20-14:50 |                          | CANCELLED                                                                               |                                                                              |
| 14:50-15:10 | Cao Xiao Lin         | *Multi-physics petascale simulations using JASMIN infrastructure*                        | Institute of Applied Physics and Computational Mathematics (China)           |
| 15:10-15:30 | Keizo Fujimoto       | *AMR-PIC simulation of collisionless magnetic reconnection*                              | National Astronomical Observatory of Japan (Japan)                           |
| 15:30-15:50 | Shu Takagi           | *Numerical simulation of the platelets adhesions on an injured vessel wall in the presence of red blood cells* | University of Tokyo (Japan)                                                  |

### Bio-computing (October 18th)

| Time     | Speaker               | Title                                                                                   | Institution                                                                 |
|----------|-----------------------|-----------------------------------------------------------------------------------------|------------------------------------------------------------------------------|
| 13:50-14:20 | Leonardo Guidoni    | *Tackling the electron correlation in biomolecules by Quantum Monte Carlo / Molecular Mechanics* | University of L’Aquila (Italy)                                               |
| 14:20-14:50 | Kaori Fukuzawa      | *Development and application of ab-initio fragment molecular orbital method for bio-macromolecules* | Mizuho Information & Research Institute Inc. (Japan)                         |
| 14:50-15:10 | Chi-Tin Shih        | *Structural and functional analysis of the drosophila brain network*                     | Tunghai University (Taiwan)                                                  |
| 15:10-15:30 | Busara Pattanasiri  | *Thermodynamics and structural behavior of a confined HP protein determined by Wang-Landau sampling* | Mahidol University (Thailand)                                                |
| No. | Full Name               | Affiliation                                      | Country     | Title                                                                 | Poster Session Details |
|-----|------------------------|--------------------------------------------------|-------------|----------------------------------------------------------------------|------------------------|
| 1   | Baumeister Paul F.     | PGI & IAS, JARA                                  | Germany     | juRS - Massively Parallel DFT Calculations in Real-Space             | Poster Session        |
| 2   | Bernardes Americo      | Universidade Federal de Minas Gerais             | Brazil      | Computer simulation of InAs HEMTs considering strain and Quantum    | Poster Session        |
| 3   | Bobrowski Maciej        | Gdansk University of Technology                  | Poland      | Reduction of metal films and chemical vapor deposition of polymers  | Poster Session        |
| 4   | Chen Kuan Peng         | National Center for High-Performance Computing   | Taiwan      | Quantum-Algebra Partition and Quantum Error-Correction Codes          | Poster Session        |
| 5   | de Doncker Elise H.    | Western Michigan University                      | USA         | Fluid simulation of plume head-on collision dynamics during pulsed laser | Poster Session        |
| 6   | Endoh Akira            | Fujitsu Laboratories Ltd./NICT                   | Japan       | Monte Carlo simulation of InAs HEMTs considering strain and Quantum | Poster Session        |
| 7   | Endo H.                | Hokkaido University                             | Japan       | Fluid simulation of plume head-on collision dynamics during pulsed laser | Poster Session        |
| 8   | Fauzi Umar             | Faculty of Mathematics and Natural Sciences, ITB | Indonesia   | Computer simulation of InAs HEMTs considering strain and Quantum    | Poster Session        |
| 9   | Freza Sylwia           | Gdansk University of Technology                  | Poland      | Reduction of metal films and chemical vapor deposition of polymers  | Poster Session        |
| 10  | Fujii Risa              | International Centre for High-Performance Computing | Japan       | Monte Carlo simulation of InAs HEMTs considering strain and Quantum | Poster Session        |

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| 36  | Effect of Chemical Kinetics of a Planar Atmosphere-Pressure N2/O2/NH3 | J. Kim                                                 | Chiao Tung University, Taiwan                                              |
| 37  | A Mechanistic Study of Photodissociation of Graphene                 | H. Ishida                                              | Kyung Hee University, Republic of Korea                                    |
| 38  | Exact Partition Function Zeros of a Polymer on a Square Lattice      | T. Ishida                                              | Soongil University, Republic of Korea                                      |
| 39  | Characteristics of Seismic Networks in Spatial Scales                | J. Kim                                                 | Kyung Hee University, Republic of Korea                                    |
| 40  | Analysis of Thermal Conductivity of Largescale Low Temperature        | P. Kaurav                                               | Govt. Holkar Science College, India                                        |
| 41  | Numerical Study of Electron Acceleration by a Magnetized Plasma Wave | F. Kaurav                                               | Kharazmi University, Iran                                                  |
| 42  | MHD Simulations of Compressible Supersonic Turbulence in Galaxy Cluster-like | J. Lee                                                 | Kyung Hee University, Republic of Korea                                    |
| 43  | High Pressure Multi-Valance Quantum Calculations for One-Dimensional Hubbard Model | S. Lee                                                 | Kyung Hee University, Republic of Korea                                    |
| 44  | Very High Precision Determination of Low-Energy Parameters: The 2d-Phosphodiapsis | K. Kargarian                                           | Kharazmi University, Iran                                                  |
| 45  | A Non-Maxwellian Tensor Approach to Photodissociation for Phosphodiapsis and Asymmetric Exclusion Process | P. Kaurav                                               | Kyung Hee University, Republic of Korea                                    |
| 46  | A Population Monte Carlo Estimation of the Current Distribution of an Abolition | F. Li                                                  | Soongil University, Republic of Korea                                      |
| 47  | MHD Simulations of Compressible, Supersonic Turbulence in Galaxy Cluster-like | J. Lee                                                 | Kyung Hee University, Republic of Korea                                    |
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| 24   | Li Zhi  | Yukawa Institute for Theoretical Physics, Kyoto University | Spin Density Wave in Chromium under High Pressure |
| 25   | Lin Paoan | National Tsing Hua University | Band structure of zigzag graphene nanoribbon with DFT calculation |
| 26   | Liu Yun-Ping | Department of Physics, National Taiwan University | New Half-metallic Materials Study on Double Perovskite Sr2Bi2OB6 (Bi=B and Fe) |
| 27   | Madkour Tarek M. | The American University in Cairo | Conformational analysis investigation into the influence of nano-porosity of multilayered porous graphene on intrinsic gas permeability and binding of hydrophobic analytes |
| 28   | Matsushita Katsuyoshi | Graduate School of Engineering, Osaka University | Theory of electric transport in helical polyacetylene using quantum Monte Carlo |
| 29   | Mayes Maricris L | Argonne National Laboratory | Towards Large Scale Fully Ab Initio Calculations Using Fragment Molecular Orbital Method on Mira (Blue Gene/Q) |
| 30   | Medina Stefan | University of Mainz, Germany | A mesoscopic simulation method for photovoltaics at high cell efficiencies |
| 31   | Minoshima Takashi | JAMSTEC, Japan | Optimization of the Jastrow factor in the correlated wave function of electrons using the first-principles transcorrelated method for solid-state calculations |
| 32   | Mitsutake Kunitio | Frontier Research Center, Canon Inc. | Monitoring multi-dimensional distributions for visual simulations of molecular processes |
| 33   | Nguyen Huy Duy | Graduate School of Engineering, Osaka University | Transport properties of boron carbide nitride hetero-nanotubes |
| 34   | Ochi Masayuki | Department of Physics, The University of Tokyo | Multi-moment advancement scheme for Vlasov simulations of magnetized plasma |
| 35   | Ono Youky | The University of Tokyo | First-Principles Molecular Dynamics Simulations for Graphene Growth Process on Si-terminated (0001) Surface |
| 36   | Purohit Ghanshyam | Sir Padampat Singhania University, Udaipur, India | Calculation of triple differential cross section for the electron impact ionization of noble gas targets |
| 37   | Rafiee Dastjerdi Somayeh | Shahid Beheshti University, Iran | Finite difference time domain method for calculating the band structure of 2D photonic crystals and near-infrared imaging |
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| 38   | Sako Tokuei               | Nihon University                                                                         | Japan       | Fermi- and conjugate-Fermi hole analyses in two-electron atomic systems     |
| 39   | Salam Tejeshwori          | NEHU India                                                                                 | India       | Computational calculation of alkyltransferase of alkylated mutagenic DNA bases |
| 40   | Sano Takayoshi            | Osaka University                                                                          | Japan       | Magnetic Field Amplification Associated with the Nonlinear Growth of Richtmyer-Meshkov Instability |
| 41   | Sharma Uttam              | Shri Vaishnav Institute of Technology and Science, Indore                                  | India       | Development of tungsten coatings and characterization under plasma operations in ADITYA limiter tokamak and in future SST-1 diverter tokamak |
| 42   | Shinjo Kazuya             | Yukawa Institute for Theoretical Physics, Kyoto                                             | Japan       | Dynamical DMRG Study of Spin Excitations in Disordered Spin-Peierls Systems |
| 43   | Skurski Piotr             | Gdansk University                                                                         | Poland      | Reactivity of paraffins with substituted vinyl molecules                      |
| 44   | Su Wei Chih               | National Center for High-performance Computing                                             | China       | Modeling Migration in Multilayer Polymer Systems by a Finite Difference Method |
| 45   | Takeuchi Yasushi          | National Institute for R&D, Isotopic and Molecular Technologies, Cluj-Napoca              | Romania     | A Dynamical Study with Applications of the Pebble Game Algorithm              |
| 46   | Teng Ping-Han             | National Tsing Hua University                                                             | Taiwan      | Development of Method for Hordesch's 2X4 System                              |
| 47   | Tosa Valer                | National Institute for R&D, Isotopic and Molecular Technologies, Cluj-Napoca              | Romania     | A Graph Theoretical Approach to Fluctuating Networks in Glass-Forming Liquids: A Novel Parameter by Instantaneous Normal Mode Analysis for Melting Behaviour |
| 48   | Tröster Andreas           | Vienna University                                                                         | Austria     | Monte Carlo Simulation of Curved Interface Free Energies                      |
| 49   | Wang Kaier                | School of Engineering, The University of Waikato                                           | New Zealand  | Underlying mechanisms for the slow oscillation observed in nonrelm sleep      |
| 50   | Wang Z.                   | Advanced Manufacturing Research Institute, Tsing Hua University                            | China       | Magnetic Field Amplification Associated with the Nonlinear Growth of Richtmyer-Meshkov Instability |
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| 53   | Zhou H.                   | National University of Defense                                                             | China       | Computational calculation of alkyltransferase of alkylated mutagenic DNA bases |
| 54   | Zhou J.                   | National University of Defense                                                             | China       | Computational calculation of alkyltransferase of alkylated mutagenic DNA bases |
| 55   | Zhou Y.                   | National University of Defense                                                             | China       | Computational calculation of alkyltransferase of alkylated mutagenic DNA bases |
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| 57   | Zhang J.                  | National University of Defense                                                             | China       | Computational calculation of alkyltransferase of alkylated mutagenic DNA bases |
| 58   | Zhang S.                  | National University of Defense                                                             | China       | Computational calculation of alkyltransferase of alkylated mutagenic DNA bases |
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| 50  | Abdul Aleem       | King Abdul Aziz University           |                                                                      |
| 51  | Watanabe Takeshi  | Department of Scientific Simulations, Nagoya Institute of Technology, Japan | Kinetic energy spectrum of the low Reynolds number turbulence with polymer |
| 52  | Wilms Johannes    | University of Vienna, Austria         | Advances in Thermocapillary Droplet Migration                          |
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| 55  | Yamaneaka Masanori| Tokyo Institute of Technology, Japan  | Numerical study of topological crossover of protein Genus            |
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| 62  | Komatsu Takeo     | Tokyo Institute of Technology, Japan  |                                                                      |
| 63  | Komiyama Hideo    | Tokyo Institute of Technology, Japan  |                                                                      |
| 64  | Kondo Kenji       | Tokyo Institute of Technology, Japan  |                                                                      |
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| 78  | Kondo Kenji       | Tokyo Institute of Technology, Japan  |                                                                      |
| 79  | Kondo Kenji       | Tokyo Institute of Technology, Japan  |                                                                      |
| 80  | Kondo Kenji       | Tokyo Institute of Technology, Japan  |                                                                      |
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| 58  | Chau Shiu-Wu | National Taiwan University of Science and Technology | Taiwan | Thermal Plasma Flow Modeling of Non-Transferred Steam Torch Using a Non-Equilibrium Approach |
| 59  | Cho Kihyeon | KISTI | Republic of Korea | Belle-Eq-related Particle Model for Poor Solvent |
| 60  | Fujimura Takayoshi | The Institute of Scientific and Industrial Research, Osaka University | Japan | Stable arrangement of impurities of copper in silicon |
| 61  | Fukushima Akinori | Tohoku University | Japan | Molecular dynamics simulation of water drop in micro pores |
| 62  | Hanaoka Kyohei | Graduate School of Pure and Applied Sciences, University of Tsukuba | Japan | QM/MM simulation revealed a substrate mediated proton relay mechanism in DNA religation reaction catalyzed by Type II DNA topoisomerase |
| 63  | Iwata Ryosuke | Graduate school of engineering, Gifu University | Japan | Effect of atomic adsorption of catalytic metals on mechanical properties of graphene |
| 64  | Kawaguchi Kazutomo | Kanazawa University | Japan | Free energy profile of Hsp90-ADP binding by molecular dynamics simulations |
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| 66  | Kim Kyungsik | Pukyong National University | Republic of Korea | Dynamical mechanism of the scaling behavior in multifractal structures |
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| 70  | Lee Kyungmoon | Kyungpook National University | Korea | Computational simulation of flow in double curved vascular model: A test on the accuracy of theoretical models on the fluid dynamics |
| 71  | Li Chao | Beijing Institute of Technology | China | Hybrid Method for Modeling of Non-Transferred Steam Torch Using a Non-Equilibrium Approach |
| 72  | Liu Bin | Key Lab of Material Science and Technology, National Taiwan University of Science and Technology | Taiwan | Hybrid Functional Study on Diffusion in Silicate Cathode Material Li2NiO3 |

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| 71   | Compatibility-based evolution of bipartite networks and its connectivity and topological overlap patterns | Maeng SeongEun, Inha University, Dept of Physics, Republic of Korea   |
| 84   | Quantum Monte Carlo Simulation of Bose-Fermi Mixtures in One-Dimensional Incommensurate Optical Lattices | Masaki Akiko, Institute for Solid State Physics, University of Tokyo, Japan |
| 77   | GPU-Accelerated MD Simulation for Short-Range Particle Interaction | Matsumoto Kosuke, Department of Physics, Kyushu University, Japan     |
| 80   | Two-Dimensionaial AMR-PIC Simulation on Solar Wind Interaction with WIND | Miki Yohei, University of Tsukuba, Japan                               |
| 83   | Hunting a Wandering Black Hole in M31 Halo Using GPU Cluster         | Mima Toshiki, Department of Mechanical Engineering, University of Tokyo, Japan |
| 84   | Mean-Field calculations including proton-neutron mixing in atomic nuclei | Noda Masashi, Institute for Molecular Science, Japan                   |
| 85   | Wave-packet dynamics in rigid bilayer graphene with thin film binding model | Nakatsukasa Takashi, RIKEN Nishina Center, Japan                       |
| 78   | Molecular dynamics simulation of gas-water transition of water in nanopores with controlled wettability | Nishida Keisuke, Kyoto University, Japan                               |
| 76   | Hunting a Wandering Black Hole in M31 Halo Using GPU Cluster         | Ohtani Hiroaki, National Institute for Fusion Science, Japan           |
| 81   | The role of a plasmoid ejection in 3-dimensional Magnetohydrodynamic simulation of solar flare | Otsuka Yuichi, RIKEN Quantitative Biology Center, Japan                |
| 79   | Mean-Field calculation including proton-neutron mixing in atomic nuclei | Otsuka Takao, Quantitative Biology Center (QBiC), Japan                |
| 82   | Two-Dimensionaial AMR-PIC Simulation on Solar Wind Interaction with WIND | Otsuka Takao, Quantitative Biology Center (QBiC), Japan                |
| 74   | Quantum Monte Carlo Simulation of Bose-Fermi Mixtures in One-Dimensional Incommensurate Optical Lattices | Physicals, University of Korea, Dept of Physics, Republic of Korea   |
| 72   | Complementarity-based evolution of bipartite networks and its connectivity and topological overlap patterns | Lee Hanjo, YITP, Kyung Hee University, Korea, South Korea             |
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- Ab Initio Study on Adsorption of Gas Molecules on Graphene Nanoribbons
- Development of a portable AMR module for various numerical simulations
- Parallel efficiency and recent progress of a linear-scaling DFT code CONQUEST
- Interaction with streaming plasma
- Development of a scalable PIC simulator and its application to spacecraft
- Plasma particle-in-cell simulation with Monte-Carlo QED reactions on pair production experiment using high-Z target
- Agent-based wealth exchange dynamics and power-law distribution of the wealth
- Numerical simulation of primordial vorticity generation by relativistic effect
- Hamiltonian dynamical structure of the Reduced MHD applied to the numerical simulation
- Effect of device geometry on current injection from metal electrodes to graphene: DFT-NEGF calculations
- Graphene: DFT-NEGF calculations
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