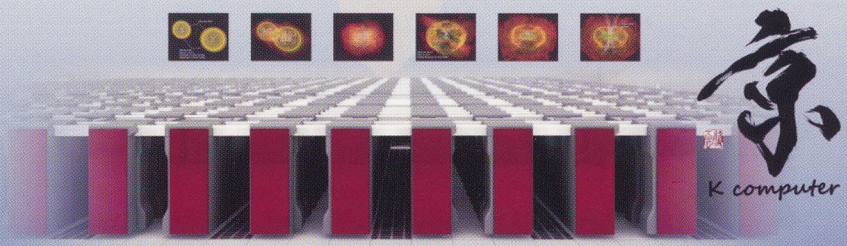
Conference on Computational Physics (CCP2012)

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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Journal of Physics: Conference Series **454** (2013) 011001 doi:10.1088/1742-6596/454/1/011001

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)

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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.

Congratulation of this important conference and wish you a great success of the conference. Please also enjoy Japan.

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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 oversea 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.

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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 Choudharys** (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 (κ) and increase in thermoelectric power (S) by embedding ErAs nanoparticles in $In_{0.53}Ga_{0.47}As$ 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 (y_i), which is a chemical index of the bond nature, and the third-order NLO polarizability (second hyperpolarizability, γ) of open-shell singlet systems. We studied the topological dependence of diradical character and second hyperpolarizability (γ) 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 (y_i=0), intermediate open-shell ($0<y_i<1$), and almost pure open-shell compounds ($y_i \cong 1$). 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 $\mathbf{C_{20}}$, $\mathbf{C_{60}}$, and $\mathbf{C_{70}}$, whereas fullerenes $\mathbf{C_{26}}$ and $\mathbf{C_{36}}$ and $\mathbf{C_{30}}$, $\mathbf{C_{40}}$, $\mathbf{C_{42}}$, and $\mathbf{C_{48}}$ are pure and intermediate open-shell compounds, respectively. Interestingly, the γ_{zzzz} enhancement ratios between $\mathbf{C_{30}}$/$\mathbf{C_{36}}$ and $\mathbf{C_{40}}$/$\mathbf{C_{60}}$ are 4.42 and 11.75, respectively, regardless of the smaller π-conjugation size in $\mathbf{C_{30}}$ and $\mathbf{C_{40}}$ than in $\mathbf{C_{36}}$ and $\mathbf{C_{60}}$. Larger γ_{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 γ_{zzzz} density analysis shows that the large positive contributions originate from the large γ_{zzzz} 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 o*ff* 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 (AAPPS)
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

1990 - Amsterdam, the Netherlands
1989 - Boston, USA

CCP2012 Committees

Chair:

Hideaki Takabe (Osaka University, Japan)

Vice-Chairs: (representatives from three regions of the world)

Kimihiko Hirao (RIKEN, (AICS), Kobe, Japan)
Michele Parrinello (ETH, Zürich, Switzerland)
Robert Rosner (University of Chicago, USA)

Scientific secretary:

Luca Baiotti (Osaka University, Japan)

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Ewald Müller (MPI for Astrophysics, Germany)
Haruki Nakamura (Osaka University, Japan)
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Stefano Sanvito (Trinity College Dublin, Ireland)
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Sandro Sorella (SISSA, Italy)
Toshikazu Takada (MEXT, Japan)
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Shinji Tsuneyuki (University of Tokyo, Japan)
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)
Vice-chair: Hideyuki Usui (Kobe University)

Luca Baiotti (Osaka University)
Atsushi Hosaka (Osaka University)
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Hideaki Takabe (Osaka University)
Shigenori Tanaka (Kobe University)
Seiichiro Ten-no (Kobe University)
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.

Booths

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
9:00		Opening ceremonies	Plenary: Zhu	Plenary: Okuda	Plenary: Arsuaga
9:45		Plenary: Imada	Plenary: Pietrucci	Plenary: Pourtois	Plenary: Rezzolla
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		Parallel sessions	Parallel sessions	Parallel sessions	Parallel sessions
16:00	Registration (starting at 15:00) and reception (starting at 17:00)	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 Renormaliz. 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	Bio-computing	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						
9:45-10:30	**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)							
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**
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 C)						
16:45-17:30	Visit to K computer (group D)						
19:00-21:00	Banquet						

Oct. 17 (Wed)							
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**
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)						

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	**Bio-computing**	**Monte Carlo methods**	**Multi-hierarchy methods**	**Molecular dynamics**	**Finite-difference, finite-volume, finite-element methods**	**Density Functional Theory**	**Particle methods**
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
16:00-16:20	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)	
Location: Kobe University, Convention Hall, 2nd floor	Chairperson: Masatoshi Imada
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 ...)	
Location: Nichii Gakkan Conference Center, 2nd floor, room 2	Chairperson: Naoki Kawashima
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)	
Location: Nichii Gakkan Conference Center, 3rd floor, hall A	Chairperson: Ritoku Horiuchi
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
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
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
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)	
Location: Nichii Gakkan Conference Center, 3rd floor, hall B	Chairperson: Ian Hawke
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)	
Location: Nichii Gakkan Conference Center, 2nd floor, room 3	Chairperson: Anatoly Spitkovsky
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)	
Location: Nichii Gakkan Conference Center, 2nd floor, room 1	Chairperson: Ivana Savic
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)	
Location: Kobe University, Convention Hall, 2nd floor	Chairperson: Michele Casula
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)	
Location: Nichii Gakkan Conference Center, 2nd floor, room 2	Chairperson: Takashi Nakatsukasa
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)**	
Location: Nichii Gakkan Conference Center, 3rd floor, hall A	Chairperson: Michael Marty Marinak
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)	
Location: K-computer building (AICS), seminar room, 1st floor	Chairperson: Hideaki Fujitani
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)	
Location: Nichii Gakkan Conference Center, 2nd floor, room 1	Chairperson: Thomas Papenbrock
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,*

	Korean Institute of Science and Technology Information (Republic of Korea)

Monte Carlo methods (October 17th)	
Location: Nichii Gakkan Conference Center, 2nd floor, room 3	Chairperson: Lev N. Shchur
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. Bridgwater**, *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
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
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**, P*ore space characterization and fluid flow properties estimation of digital porous materials,* Institut Teknologi Bandung (Indonesia)

Visualization (October 17th)	
Location: Kobe University, Convention Hall, 2nd floor	Chairperson: Hiroaki Ohtani
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)	
Location: Nichii Gakkan Conference Center, 2nd floor, room 2	Chairperson: Ian Hawke
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)**	
Location: Nichii Gakkan Conference Center, 3rd floor, hall A	Chairperson: Michael Norman
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

October 18th (Thursday)

Finite-difference, finite-volume, finite-element methods (October 18th)	
Location: Nichii Gakkan Conference Center, 3rd floor, hall B	Chairperson: Luciano Rezzolla
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)	
Location: Nichii Gakkan Conference Center, 2nd floor, room 3	Chairperson: Hideyuki Usui
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,* 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)	
Location: Nichii Gakkan Conference Center, 2nd floor, room 1	Chairperson: Masaharu Isobe
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)	
Location: Kobe University, Convention Hall, 2nd floor	Chairperson: Werner Krauth
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)	
Location: Nichii Gakkan Conference Center, 2nd floor, room 2	Chairperson: Stefan Blügel
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	**NguyenTien 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)	
Location: Nichii Gakkan Conference Center, 3rd floor, hall A	Chairperson: Ryoichi Yamamoto
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)	
Location: K-computer building (AICS), seminar room, 1st floor	Chairperson: Fabio Pietrucci
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)

Poster sessions

MONDAY 15					
N.	SURNAME	NAME	AFFILIATION	COUNTRY	TITLE
1	Baumeister	Paul F.	PGI & IAS, FZ Julich, JARA	Germany	juRS - Massively Parallel DFT calculations in Real-Space
2	Bernardes Tristao	Americo	Universidade Federal de Ouro Preto	Brazil	Computer simulation of direct iron reduction
3	Bobrowski	Maciej	Gdansk University of Technology	Poland	Reduction of metal salts and chemical vapour deposition of parylenes
4	Chen	Kuan Peng	National Center For High-performance Computing, National Applied Research Laboratories	Taiwan	Quotient-Algebra Partition and Quantum Error-Correction Codes
5	Chiu	Pao-Hsiung	National Center for High-Performance Computing	Taiwan	GPU implementation for the flux-splitting Maxwell's equations solver
6	Choudhary	Kamal Kumar	Shri Vaishnav Institute of Technology and Science, Indore	India	Quantitative analysis of thermoelectric properties of crystalline semiconductors embedded with ErAs nanoparticles
7	de Doncker	Elise H.J.	Western Michigan University	USA	Shared memory iterated numerical integration for Feynman loop integrals
8	Endoh	Akira	Fujitsu Laboratories Ltd./NICT	Japan	Monte Carlo Simulation of InAs HEMTs Considering Strain and Quantum Confinement Effects
9	Fauzi	Umar	Faculty of Mathematics and Natural Sciences, Institut Teknologi Bandung	Indonesia	Computer rock model to study influence of clays and lamina on fluid permeability
10	Freza	Sylwia	Gdansk University of Technology	Poland	Parylene copolymerization
11	Fujii	Risa	Kobe University	Japan	Fluid simulation of plume head-on collision dynamics during pulsed laser

12	Hieida	Yasuhiro	Computer and Network Center, Saga University	Japan	A population Monte Carlo estimation of the current distribution of an asymmetric exclusion process
13	Ishida	Toshimasa	Fukui Institute for Fundamental Chemistry, Kyoto University	Japan	A Non-adiabatic Trajectory Approach to Photoisomerization for Rhodopsin and Isorhodopsin. The Origin of Faster and More Efficient Isomerization in Rhodopsin
14	Jiang	Fu-Jiun	Physics Department, National Taiwan Normal Universiy, Taipei	Taiwan	Very High Precision Determination of Low-Energy Parameters: The 2-d Heisenberg Quantum Antiferromagnet as a Test Case
15	Jones	Thomas W	University of Minnesota	USA	MHD simulations of compressible, subsonic turbulence in galaxy cluster-like environments
16	Kaneko	Ryui	Department of Applied Physics, University of Tokyo	Japan	High-Precision Multi-Variable Variational Calculations for One-Dimensional Hubbard Model
17	Kargarian	Ameneh	Kharazmi University	Iran	Numerical study of electron acceleration by a magnetized Plasma wave
18	Kaurav	Netram	Department of Physics, Govt. Holkar Science college	India	Analysis of thermal conductivity of LaFeAsO at low temperature
19	Kim	Kyungsik	Pukyong National University	Republic of Korea	Characteristics of seismic networks in spatial scales
20	CANCELLED				
21	Lee	Jae Hwan	Soongsil Unviersity	Republic of Korea	Exact partition function zeros of a polymer on a square lattice
22	Lee	Seongsik	kyung hee university	Republic of Korea	A Mechanistic Study of Fluorination of Graphene
23	Li	FuLi	Department of Mechanical Engineering, National Chiao Tung University	Taiwan	One-Dimensional Fluid Modeling of a Planar Atmospheric-Pressure N2/O2/NH3 Dielectric Barrier Discharge with Reduced Chemical Kinetics

24	Li	Zhi	Yukawa Institute for Theoretical Physics, Kyoto University	Japan		Spin Density Wave in Chromium under High Pressure
25	Lin	Paoan	National Tsing Hua University	Taiwan	Taiwan	Band structure of zigzag graphene nanoribbon with DFT calculation
26	Liu	Yun-Ping	Department of Physics, National Taiwan University	Taiwan	Taiwan	New Half-metallic Materials Study on double perovskite Sr2ZnBO6 (B=Tc and Re)
27	Madkour	Tarek M.	The American University in Cairo	Egypt	Egypt	Conformational analysis investigation into the influence of nano-porosity of ultra-permeable ultra-selective polyimides on its diffusivity as potential membranes for use in the "green" separation of natural gases
28	Matsushita	Katsuyoshi	Cybermedia Center, Osaka University	Japan	Japan	Multicanonical Simulation of Coupled Folding and Binding of Intrinsically Disordered Protein on an Ising-like Protein Model
29	Mayes	Maricris L	Argonne National Laboratory	USA	USA	Towards Large Scale Fully Ab Initio Calculations Using Fragment Molecular Orbital Method on Mira (Blue Gene/Q)
30	Medina	Stefan	University of Mainz	Germany	Germany	A mesoscale simulation method for polyelectrolytes at high salt concentrations
31	Minoshima	Takashi	JAMSTEC	Japan	Japan	Multi-moment advection scheme for Vlasov simulations of magnetized plasma
32	Mitsutake	Kunihiro	Frontier Research Center, Canon Inc.	Japan	Japan	Theory of electric transport in helical polyacetylene - a multipath pi-electron system
33	Nguyen	Huy Duy	Graduate School of Engineering, Osaka University	Japan	Japan	Transport properties of boron carbide nitride hetero-nanotubes
34	Ochi	Masayuki	Department of Physics, The University of Tokyo	Japan	Japan	Optimization of the Jastrow factor in the correlated wave function of electrons using the first-principles transcorrelated method for solid-state calculations
35	Ono	Youky	The University of Tokyo	Japan	Japan	First-Principles Molecular Dynamics Simulations for Graphene Growth Process on Stepped SiC(0001) Surface
36	Purohit	Ghanshyam	Sir Padampat Singhania University, Udaipur	India	India	Calculation of triple differential cross section for the electron impact ionization of noble gas targets
37	Rafiee Dastjerdi	Somayeh	Shahid Beheshti University	Iran	Iran	Finite difference time domain method for calculating the band structure of 2D photonic crystal lens and near-infrared imaging

38	Sako	Tokuei	Nihon University	Japan	Fermi- and conjugate-Fermi hole analysis in two-electron atomic systems	
39	Salam	Tejeshwori	NEHU	India	Computational calculation on 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 University	Japan	Dynamical DMRG Study of Spin Excitations in Disordered Spin-Peierls Systems	
43	Skurski	Piotr	Gdansk University of Technology	Poland	Reactivity of parylene with substituted vinyl molecules	
44	Su	Wei Chih	National Center for High-performance Computing	Taiwan	One decomposition method for Hordecki's 2X4 system	
45	Takeuchi	Yasushi	Hinode Science Center, National Astronomical Observatory of Japan	Japan	A graph theoretical approach to fluctuating networks in glass-forming liquids: A molecular dynamics study with applications of the pebble game algorithm	
46	Tang	Ping-Han	National Chiao Tung University	Taiwan	Order parameter by instantaneous normal mode analysis for melting behaviour of cluster Ag17Cu2	
47	Tosa	Valer	National Institute for R&D Isotopic and Molecular Technologies, Cluj-Napoca	Romania	Modelling migration in multilayer polymer systems by a finite difference method	
48	Tröster	Andreas	Vienna University of Technology Wiedner Hauptstrasse 8-10/136 A-1040 Wien	Austria	Monte Carlo Simulation of Curved Interface Free Energies	
49	Wang	Kaier	School of Engineering, The University of Waikato, Hamilton	New Zealand	Underlying mechanism for the slow oscillation observed in nonREM sleep, general anesthesia and generalized seizure	

50	Wardak	Khaleda Abdul Aleem	King Abdul Aziz University	Saudi Arabia	Investigation of solid state emission of a Cu(I) Br Complex using ab initio method
51	Watanabe	Takeshi	Department of Scientific and Engineering Simulations, Nagoya Institute of Technology	Japan	Kinetic energy spectrum of the low Reynolds number turbulence with polymer additives
52	Wilms	Johannes	University of Vienna	Austria	Mutual information as a tool to study correlations and phase transitions
53	Wu	Z-B	Chinese Academy of Sciences	China	Advances in Thermocapillary Droplet Migration
54	Yamada	Yuta	Osaka Institute of Technology	Japan	Numerical Study of 5-dimensional Gravitational Collapses
55	Yamanaka	Masanori	College of Science and Technology, Nihon University	Japan	Numerical study of topological crossover of protein genus
56	Yasuda	Hiroaki	National Institute of Information and Communications Technology	Japan	Non-equilibrium Green's function calculations of terahertz-quantum cascade lasers for room-temperature operations

TUESDAY 16

N.	SURNAME	NAME	AFFILIATION	COUNTRY	TITLE
57	Bui	Kieu My Thi	NIMS	Japan	Hybrid Functional Study on Diffusion in Silicate Cathode Material Li2NiSiO4
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 II Data Handling System
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 droplet 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
65	Kawatsu	Tsutomu	Institute for Molecular Science	Japan	A Tunnel Pathway Analysis using the Semi-classical Instanton Approach
66	Kim	Kyungsik	Pukyong National University	Republic of Korea	Dynamical mechanism of the scaling behavior in multifractal structures
67	Kinjo	Tomoyuki	Toyota Central R&D Labs., Inc.	Japan	Coarse-grained Particle Model for Polar Solvent
68	Kirihara	Takanobu	University of Tsukuba	Japan	Resolving the outer density profile of dark matter halo in Andromeda galaxy
69	Kodera	Mitsuru	National Institute for Materials Science	Japan	First-principles study for initial stage of graphene nucleation at the step on SiC
70	Lee	Kyungeun	RIKEN	Japan	Computational simulation of flow in double curved vascular model: A test on the accuracy

71	Lu	Hantao	YITP, Kyoto University	China	Photoinduced spin-order destructions in one-dimensional extended Hubbard model
72	Maeng	SeongEun	Inha University, Dept of Physics	Republic of Korea	Compatibility-based evolution of bipartite networks and its connectivity and topological overlap patterns
73	Masaki	Akiko	Institute for Solid State Physics, University of Tokyo	Japan	Quantum Monte Carlo Simulation of Bose-Fermi Mixtures in One-Dimensional Incommensurate Optical Lattices
74	Matsumoto	Kosuke	Department of Physics, Kyushu University	Japan	GPU-Accelerated MD Simulation for Short-Range Particle Interaction
75	Matsumoto	Masaharu	Kobe University	Japan	Two-Dimensional AMR-PIC Simulation on Solar Wind Interaction with Mini-Magnetosphere
76	Miki	Yohei	University of Tsukuba	Japan	Hunting a Wandering Black Hole in M31 Halo Using GPU Cluster
77	Mima	Toshiki	Department of Mechanical Engineering, University of Tokyo	Japan	Molecular dynamics simulation for vapor-liquid phase transition of water in nanocylinder with controlled wettability
78	Nakamura	Etsuko	Graduate School of Engineering, Gifu University	Japan	Wave-packet dynamics in gated bilayer graphene within Tight-Binding model
79	Nakatsukasa	Takashi	RIKEN Nishina Center	Japan	Mean-field calculation including proton-neutron mixing in atomic nuclei
80	Nishida	Keisuke	Kyoto University	Japan	The role of a plasmoid ejection in 3-dimensional magnetohydrodynamic simulation of a solar flare
81	Noda	Masashi	Institute for Molecular Science	Japan	Massively-Parallel TDDFT calculations based on Finite Difference Method in Real-time and Real-Space
82	Ohtani	Hiroaki	National Institute for Fusion Science	Japan	Data compression concepts on scientific visualization for time-series data of huge particle system
83	Otsuka	Yuichi	RIKEN	Japan	Quantum Monte Carlo study of the half-filled Hubbard model on the honeycomb lattice
84	Otsuka	Takao	RIKEN Quantitative Biology Center (QBiC)	Japan	Structure relaxation and binding energy calculations of FK506 binding protein complexes using order-N DFT code CONQUEST

85	Saito	Hiroaki	Kanazawa University	Japan	Binding Free Energy of Azurin-Cytochrome c551 Complex by all-atom Molecular Dynamics Simulation
86	Santra	Sitangshu Bikas	Department of Physics, Indian Institute of Technology Guwahati, Assam	India	Directed sandpile models on random and scale-free networks
87	Shabbir	Muhammad	Osaka University	Japan	Interplay between Diradical Characters and Third-Order Nonlinear Optical Properties in Fullerene Systems
88	Shahjahan	Mohammad	ISIR, Osaka University	Japan	Ferromagnetic half metals based on chalcopyrite semiconductors CuAlSe2 and CuInS2
89	Shiibashi	Tomohiro	Seikei university	Japan	Influence of the substitutional impurities in the electronic transportation properties of carbon nanotubes
90	Shimamura	Kohei	Department of physics Kumamoto University	Japan	Ab initio study of dissociation reaction of ethylene molecules on nickel cluster
91	Shinaoka	Hiroshi	AIST	Japan	First-principles study on noncollinear magnetism and effects of spin-orbit coupling in 5d pyrochlore oxide Cd2Os2O7
92	Shinaoka	Hiroshi	AIST	Japan	Unconventional spin-glass behaviors in pyrochlore Heisenberg antiferromagnets coupled with lattice distortions
93	Shiroto	Takashi	Department of Aerospace Engineering, Tohoku Univ.	Japan	Radiation Hydrodynamics Simulation of High-Z Doped ICF Targets
94	Shoji	Masafumi	Institute of Space and Astronautical Science	Japan	Precipitation of Highly Energetic Protons by Helium Branch Electromagnetic Ion Cyclotron Triggered Emissions
95	Sota	Shigetoshi	RIKEN AICS	Japan	Dynamical density matrix renormalization group study of high-energy optical conductivity in high-Tc copper-oxides
96	Suzuki	Takafumi	University of Hyogo	Japan	Edge state of two dimensional quantum spin systems
97	Tadano	Terumasa	Department of Physics, The University of Tokyo	Japan	First-principles studies on the reduced thermal conductivity of a clathrate Ba8Ga16Sn30
98	Tajima	Nobuo	National Institute for Materials Science	Japan	Carbon atom clustering and cluster growth in CVD graphene formation on nickel surface: A theoretical study

99	Takano	Yu	Osaka University	Japan	Density functional study of conformational preferences of intermediates and transition states in the alkaline hydrolysis of dimethyl phosphate
100	Tsuyuki	Hiroyoshi	Seikei University	Japan	Electronic transport properties in substitutionally doped graphene nanoribbons
101	Tung	JenChuan	Graduate Institude of Applied Physics, National Chengchi University	Taiwan	Spin and Anomalous Hall Conductivities in Co-based Heusler Alloys: A First-principle Study
102	Uemura	Naoki	The Institute of Scientific and Industrial Research, Osaka university	Japan	First-principles study of α-tetragonal boron
103	Usui	Hideyuki	Kobe University	Japan	Full Particle-In-Cell Simulation of Ion Beam Neutralization
104	Velechovsky	Jan	Czech Technical University	Czech Republic	Symmetry-preserving Remap of Vectors for Staggered ALE Hydrodynamics
105	Vu	Truong V.	Ritsumeikan University	Japan	Numerical simulations of solidification with volume change by a front-tracking method
106	Watanabe	Hiroshi	RIKEN	Japan	Theoretical study of novel insulating and superconducting states in Ir oxides with large spin-orbit coupling
107	Yagi	Yohei	Graduate school of System Informatics, Kobe University	Japan	Development of Parallelized Adaptive Mesh Refinement Particle in Cell with Dynamic Domain Decomposition
108	Yamamoto	Atsusi	AICS RIKEN	Japan	Superfluidity of One-dimensional Trapped Fermionic Optical Lattices with Spatially Alternating Interactions
109	Yoshimoto	Yuta	Department of Mechanical Engineering, The University of Tokyo	Japan	Construction of interaction models of dissipative particle dynamics by coarse-graining Lennard-Jones fluids: Investigation on the system with vapor-liquid interfaces
110	Zivny	Oldrich	Institute of Plasma Physics AS CR, Prague	Czech Republic	Calculation of Composition and Thermodynamic Properties of Non-Equilibrium Thermal Plasma at High Temperatures

					WEDNESDAY 17
N.	SURNAME	NAME	AFFILIATION	COUNTRY	TITLE
111	Anh	Le The	Japan advanced institute of science and technology	Viet Nam	Ab initio study of Phosphorus donor states in single dopant transistor with a stub-shaped channel
112	Belosludov	Rodion V	Institute for Materials Research, Tohoku University, Sendai	Japan	Realization of Gas Storage Materials based on Clathrate Hydrate: Computational Modelling
113	Blümer	Nils	Johannes Gutenberg University Mainz	Germany	Momentum-dependent pseudogaps in the half-filled two-dimensional Hubbard model
114	Bouamama	Khellil	Univesity Ferhat Abbas of Setif, Algeria	Algeria	Ab-initio calculation of the photoelastic constants of SiC
115	Calcavecchia	Francesco	Johannes Gutenberg Universitat, MAINZ Graduate School	Germany	Variational Approach to Hydrogen's Electronic Structure
116	Chakraborty	Himanshu	Department of Physics, Indian Institute of Technology Bombay	India	Large Scale Configuration Interaction Calculations of Linear Optical Absorption of Octacene, Nonacene and Decacene
117	Chen	Chih-Huan	Department of Physics and Center for Theoretical Sciences, National Taiwan University	Taiwan	Spin-spiral waves in zigzag 3d transition metal atomic chains from first principle calculations
118	Chen	Chun-Nan	National Chiao Tung University	Taiwan	Multi-Objective Solar Cell Design Optimization Using Semiconductor Device Simulation-Based Evolutionary Algorithm
119	Chen	Tingting	Hiroshima University	Japan	Empirical Study of the GARCH model with Rational Errors
120	Chetty	Nithaya	University of Pretoria, South Africa	South Africa	The African School of Electronic Structure Methods and Applications

121	Chouakri	Sid Ahmed	Laboratoire de Telecommunications et Traitement Numerique du Signal, University of Sidi Bel Abbes	Algeria	Wavelet Transform and Huffman Coding Based ECG compression Algorithm: Application to Telecardiology
122	Doi	Shotaro	Department of Physics, Graduate School of Science, Osaka University	Japan	Development of first-principles electronic structure calculation code for large super cell systems by using screened KKR method
123	Fujii	Tetsuya	Dept. of Micro Eng. Kyoto University	Japan	Energy analysis of a cofilin-decorated actin filament using molecular dynamics simulations
124	Fujiwara	Susumu	Kyoto Institute of Technology	Japan	Shape transition of micelles in amphiphilic solution: A molecular dynamics study
125	Fukuda	Ikuo	RIKEN	Japan	A simple non-Ewald scheme: the zero-dipole summation method and its application to molecular systems
126	Heide	Marcus	Graduate School of Engineering, Osaka University	Japan	Effcient relaxation of magnetic moments in noncollinear DFT calculations
127	Higuchi	Katsuhiko	Hiroshima University	Japan	Correction method of the pair density functional theory and its application to atomic structure calculations
128	Hirokawa	Kazuya	Niigata University	Japan	Parallel-computing solutions of symmetry-unrestricted Hartree-Fock-Bogoliubov equations in the three-dimensional Cartesian-mesh representation
129	Huang	Shu-Ping	Kyushu University	Japan	DFT study of the mechanism for methane hydroxylation by soluble methane monooxygenase (sMMO): effects of oxidation state, spin state, and coordination number
130	Ikeda	Yuji	Department of Micro Engineering, Kyoto University	Japan	Perturbative Approach for Calculating Electronic Structures with Electric Currents
131	Inglis	Stephen C	University of Waterloo	Canada	Phase transition detection using Renyi entropy in classical and quantum Monte Carlo

132	Inoue	Shinri	Japan Advanced Institute of Science and Technology	Japan	Ab initio Study on Adsorption of Gas Molecules on Graphene Nanoribbons
133	Ishimoto	Yukitaka	RIKEN CDB	Japan	Two-dimensional lattice liquid models
134	Jansen	Karl	NIC, DESY Zeuthen	Germany	A first look at Quasi-Monte Carlo methods for lattice field theory problems
135	Kaneko	Tomoaki	Computational Materials Science Unit, NIMS	Japan	Effect of device geometry on current injection from metal electrodes to graphene: DFT-NEGF calculations
136	Kaneko	Yuta	Graduate School of Frontier Science, Tokyo University, Japan	Japan	Hamiltonian dynamical structure of the Reduced MHD applied to the numerical simulation
137	Kawazura	Yohei	Graduate School of Frontier Science, The University of Tokyo	Japan	Numerical simulation of primordial vorticity generation by relativistic effect
138	Koyama	Hiroshi	NIMS	Japan	Structures and electronic states of 3C- and 4H-SiC surfaces
139	Lee	Jae Woo	Department of Physics, Inha University, Incheon	Republic of Korea	Agent-based wealth exchange dynamics and power-law distribution of the wealth
140	Linh	Nguyen Van	Ritsumeikan University	Japan	Tracking large scale structure of open channel flow using POD-based Unscented Kalman Filter
141	Miyake	Yohei	Graduate School of System Informatics, Kobe University	Japan	Development of a scalable PIC simulator and its application to spacecraft interaction with streaming plasma
142	Miyazaki	Tsuyoshi	National Institute for Materials Science	Japan	Parallel efficiency and recent progress of a linear-scaling DFT code CONQUEST
143	Moritaka	Toseo	Institute for Laser Engineering, Osaka University	Japan	Plasma particle-in-cell simulation with Monte-Carlo QED reactions on pair production experiment using high-Z target
144	Nagara	Akihide	Graduate School of System Informatics, Kobe University	Japan	Development of a portable AMR module for various numerical simulations

145	Nakamura	Kazuma	The University of Tokyo, Department of Applied Physics	Japan		Massive parallelization of ab initio RPA and GW codes
146	Nakamura	Tatsufumi	Japan Atomic Energy Agency	Japan		High power gamma-ray source from laser irradiated solid target
147	Naylor	Wade	Department of Physics, Osaka University	Japan		Photon pair creation in microwave cavities with losses and infinitely coupled systems of differential equations
148	Nikbakht	Shahla	University of Queensland	Australia		Computation of Unequal Time Correlation Function for the Asymmetric Simple Exclusion Process Using Matrix Product States
149	Oda	Akifumi	Kanazawa University	Japan		Evaluations of conformational search accuracy of CAMDAS using experimental three-dimensional structures of protein-ligand complexes
150	Ogino	Yousuke	Tohoku University	Japan		Computational code of high-enthalpy flow equations with collisional-radiative processes
151	SaiToh	Akira	National Institute of Informatics	Japan		A multiprecision C++ library for matrix-product-state simulation of quantum computing
152	Sakakibara	Hirofumi	The University of Electro Communication	Japan		First principles band structure +FLEX approach to the pressure effect on Tc of the cuprate superconductors
153	Santra	Sitangshu Bikas	Department of Physics, Indian Institute of Technology Guwahati, Assam	India		Does explosive percolation occur away from the critical point?
154	Schaerf	Daniel	University Mainz	Germany		Predicting New Crystal Structures from First-Principles
155	Senami	Masato	Kyoto University	Japan		Effects of a surrounding medium of quantum systems on Rigged QED Simulation
156	Shirai	Nobu C	Graduate School of Science, Osaka University	Japan		Multicanonical simulation of the Domb-Joyce model and the Go model: new enumeration methods of self-avoiding walks
157	Shirakawa	Tomonori	RIKEN	Japan		Theoretical studies of a three-band Hubbard model with a strong spin-orbit coupling for 5d transition metal oxides Sr2IrO4

158	Takahashi	Masayuki	Department of Aerospace Engineering, Tohoku University	Japan	Hydrodynamics-Orbit Coupling Calculation for Flight Analysis of Actively Controlled Laser Vehicle
159	Takaishi	Tetsuya	Hiroshima University of Economics	Japan	Analysis of spin financial market by GARCH model
160	Tokita	Kei	Cybermedia Center, Osaka University	Japan	GPGPU simulations of 2D lattice neutral models in ecology
161	Torralba	Antonio Sanchez	Spanish National Cancer Research Centre (CNIO)	Spain	The allosteric couplings map of the meganuclease I-Dmol reveals long-range anticorrelations between the LAGLIDADG and DNA-binding moieties
162	Utsunomiya	Toshio	National Defense Academy	Japan	A Numerical Calculation Method for Frequency-Shift of a Plasma Wave Using Wave Digital Filters
163	Yamanaka	Shusuke	Osaka University	Japan	How to determine boundaries for QM/MM calculations? A guideline based on linear response function
164	Yamasaki	Takahiro	Fujitsu laboratories limited	Japan	Planewave based first-principles calculations on the 80,000 nodes K-computers: Application to SiC screw dislocations
165	Yoshimoto	Yoshihide	Tottori University	Japan	First-principles calculation combined with multicanonical simulation: application to the melting of ice
166	Yuasa	Fukuko	KEK	Japan	Acceleration of Feynman loop integrals in high-energy physics on many core GPUs

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