International workshop on numerical methods and simulations for materials design and strongly correlated quantum matters

March 24-25, 2017 Kobe, Japan

Welcome

Overview:

This workshop concentrates on a confluence of two research fields of machine learning technique and material science. Now, the material science has a chance to reap the benefit of recent advances of machine learning technology associated with the nature of multi-layer structures universally expected in the feedback feature of realistic systems. Machine learning has a possibility to produce novel methods for describing strong correlation in materials and molecules and computing properties to facilitate material design.

This workshop includes talks from both younger and more established researchers on the following three topics:

1. Lectures on fundamental aspects of machine leaning, including its history, essential idea, breakthrough and problems.
2. Lectures on global introduction of applications of machine learning in many research fields.
3. Talks on the development of theory and method for material and chemical designs by using material informatics and machine learning.
4. Talks on purely material sciences involved with complex quantum many body systems in physics, chemistry and biology.

We welcome you to join the workshop.

Organizers: Hiroshi Ueda, Seiji Yunoki, Takahito Nakajima, Takehiro Yonehara
Supported by: FOCUS Establishing Supercomputing Center of Excellence

Date and Venue

Date : Friday, March 24 - Saturday, March 25, 2017
Venue: RIKEN Advanced Institute for Computational Science (AICS)
Registration fee : Free of charge
※ A catering including drinks will be arranged in the poster session.
　　Please prepare JPY 1,000.- as the drink fee in the session if you attend it.

Speakers

Invited speakers [confirmed]:

Aurélien Decelle
  LRI, University of Paris-Sud

Bing Huang
  University of Basel

Edwin Miles Stoudenmire
  University of California, Irvine

Hieu Chi Dam
  Japan Advanced Institute of Science and Technology

Hiroshi Fujisaki
  Nippon Medical School

Jascha Sohl-Dickstein
  Google

John Parkhill
  University of Notre Dame

Juan Felipe Carrasquilla
  D-Wave Systems

Masato Okada
  The University of Tokyo and National Institute for Materials Science

Mikiya Fujii
  The University of Tokyo

Ryo Tamura
  National Institute for Materials Science

Satoru Iuchi
  Nagoya University

Yang Wei Koh Patrick
  Home researcher (physics), Singapore

Zi Yang Meng
  Institute of Physics, Chinese Academy of Sciences

Access details

✈ Kobe Airport (about 5 min., JPY 250.-)
    1) Take the Port Liner monorail and get off at the next station,
      "K Computer Mae"

✈ Osaka International Airport (about 90 min., JPY 1,330.-)
    1) Take the Osaka Airport Limousine bus to "Sannomiya" (Kobe),
      and then take the Port Liner monorail to "K Computer Mae" station.

✈ Kansai International Airport
    1) Take the free bus from Kansai International Airport to board the High-
      Speed Ferry to Kobe Airport, and then take the Port Liner monorail to
      "K Computer Mae" station. (about 40 min., JPY 1,850.-)
    2) Take the Osaka Airport Limousine bus to get "Sannomiya" (Kobe) and
      then take the Port Liner monorail to get the "K Computer Mae" station.
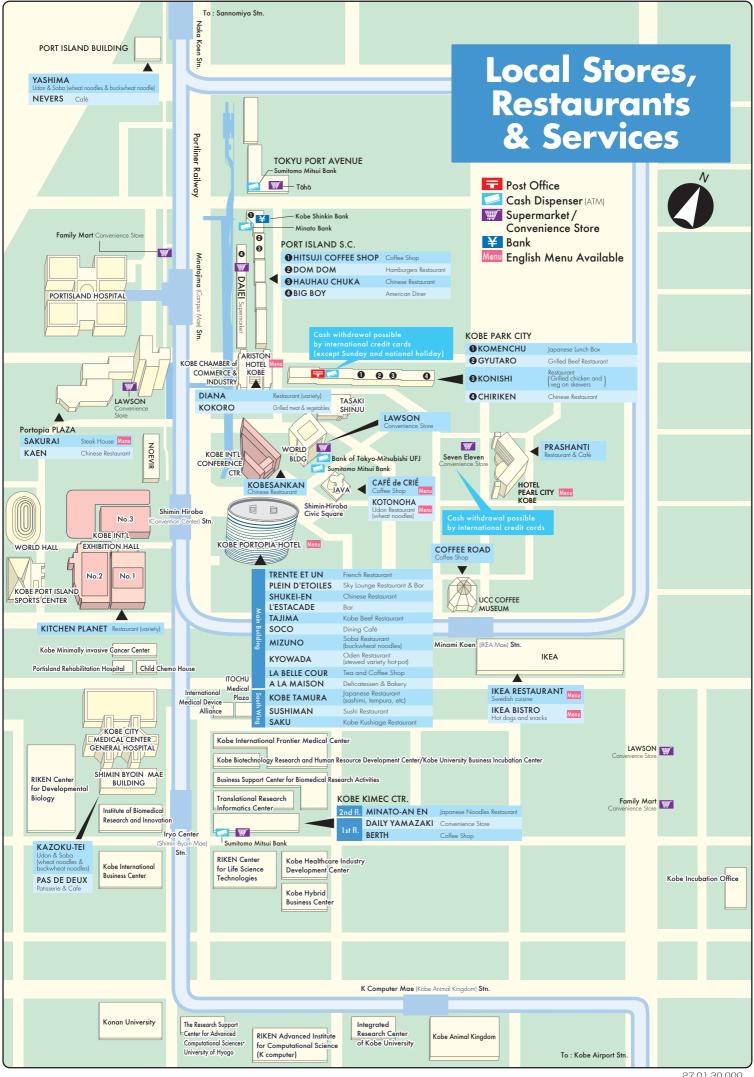   (about 100 min., JPY 2,230.-)

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Encryption method : WPA2-PSK(AES)

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For further information and help, please contact us.

Computational Molecular Science Research Team and
Computational Materials Science Research Team,
RIKEN/AICS, Kobe, Hyogo 650-0047, Japan
e-mail: kobeworkshop2016@gmail.com

Local Stores, Restaurants & Services

N

PORT ISLAND BUILDING

YASHIMA Udon & Soba (wheat noodles & buckwheat noodle)
NEVERS Café

To : Sannomiya Stn.

Naka Koen Stn.

Portliner Railway

Minatojima (Campus Mae) Stn.

Family Mart Convenience Store

PORTISLAND HOSPITAL

LAWSON Convenience Store

Portopia PLAZA
SAKURAI Steak House Menu
KAEN Chinese Restaurant

NOEVIR

WORLD HALL

No.3

KOBE INT'L EXHIBITION HALL

No.2 No.1

KOBE PORT ISLAND SPORTS CENTER

KITCHEN PLANET Restaurant (variety)

Kobe Minimally invasive Cancer Center

Portisland Rehabilitation Hospital Child Chemo House

TOKYU PORT AVENUE
Sumitomo Mitsui Bank
Tohō

Kobe Shinkin Bank
Minato Bank

DAIEI Supermarket

PORT ISLAND S.C.
❶ HITSUJI COFFEE SHOP Coffee Shop
❷ DOM DOM Hamburgers Restaurant
❸ HAUHAU CHUKA Chinese Restaurant
❹ BIG BOY American Diner

Cash withdrawal possible by international credit cards (except Sunday and national holiday)

❶ ❷ ❸ ❹

KOBE PARK CITY
❶ KOMENCHU Japanese Lunch Box
❷ GYUTARO Grilled Beef Restaurant
❸ KONISHI Restaurant (Grilled chicken and veg on skewers)
❹ CHIRIKEN Chinese Restaurant

ARISTON HOTEL KOBE Menu

KOBE CHAMBER of COMMERCE & INDUSTRY

DIANA Restaurant (variety)
KOKORO Grilled meat & vegetables

TASAKI SHINJU

LAWSON Convenience Store

KOBE INT'L CONFERENCE CTR.

WORLD BLDG

Bank of Tokyo-Mitsubishi UFJ
Sumitomo Mitsui Bank

KOBESANKAN Chinese Restaurant

JAVA

Shimin-Hiroba Civic Square

CAFÉ de CRIÉ Coffee Shop Menu
KOTONOHA Udon Restaurant (wheat noodles) Menu

Seven Eleven Convenience Store

PRASHANTI Restaurant & Café

HOTEL PEARL CITY KOBE Menu

Cash withdrawal possible by international credit cards

COFFEE ROAD Coffee Shop

UCC COFFEE MUSEUM

Shimin Hiroba (Convention Center) Stn.

KOBE PORTOPIA HOTEL Menu

Main Building	TRENTE ET UN	French Restaurant
	PLEIN D'ETOILES	Sky Lounge Restaurant & Bar
	SHUKEI-EN	Chinese Restaurant
	L'ESTACADE	Bar
	TAJIMA	Kobe Beef Restaurant
	SOCO	Dining Café
	MIZUNO	Soba Restaurant (buckwheat noodles)
	KYOWADA	Oden Restaurant (stewed variety hot-pot)
South Wing	LA BELLE COUR	Tea and Coffee Shop
	A LA MAISON	Delicatessen & Bakery
	KOBE TAMURA	Japanese Restaurant (sashimi, tempura, etc)
	SUSHIMAN	Sushi Restaurant
	SAKU	Kobe Kushiage Restaurant

Minami Koen (IKEA Mae) Stn.

IKEA

IKEA RESTAURANT Menu
Swedish cuisine

IKEA BISTRO Menu
Hot dogs and snacks

ITOCHU Medical Plaza

International Medical Device Alliance

Kobe International Frontier Medical Center

Kobe Biotechnology Research and Human Resource Development Center/Kobe University Business Incubation Center

Business Support Center for Biomedical Research Activities

Translational Research Informatics Center

KOBE KIMEC CTR.
2nd fl. MINATO-AN EN Japanese Noodles Restaurant
1st fl. DAILY YAMAZAKI Convenience Store
BERTH Coffee Shop

LAWSON Convenience Store

Family Mart Convenience Store

KOBE CITY MEDICAL CENTER GENERAL HOSPITAL

RIKEN Center for Developmental Biology

SHIMIN BYOIN MAE BUILDING

Institute of Biomedical Research and Innovation

Iryo Center (Shimin Byoin Mae) Stn.

Sumitomo Mitsui Bank

RIKEN Center for Life Science Technologies

Kobe Healthcare Industry Development Center

Kobe Hybrid Business Center

KAZOKU-TEI Udon & Soba (wheat noodles & buckwheat noodles)
PAS DE DEUX Patisserie & Cafe

Kobe International Business Center

Kobe Incubation Office

K Computer Mae (Kobe Animal Kingdom) Stn.

Konan University

The Research Support Center for Advanced Computational Sciences, University of Hyogo

RIKEN Advanced Institute for Computational Science (K computer)

Integrated Research Center of Kobe University

Kobe Animal Kingdom

To : Kobe Airport Stn.

Legend:
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- Menu English Menu Available

27.01.30.000

Program

09:30-10:00	**Registration**
	☕ **Welcome coffee (09:50-)**
10:00-10:05	Seiji Yunoki, *RIKEN AICS*
	Opening Remarks

Session 1 (Chair: Juan Felipe Carrasquilla)

10:05-10:50	Jascha Sohl-Dickstein, *Google*
	Deep Unsupervised Learning using Nonequilibrium Thermodynamics
10:50-11:35	Edwin Miles Stoudenmire, *University of California, Irvine*
	Machine Learning with Quantum-Inspired Tensor Networks
11:35-12:20	Satoru Iuchi, *Nagoya University*
	Computational study on ultrafast electronic relaxation in an iron(II) complex
12:20-13:30	🍴 **Lunch**

Session 2 (Chair: Edwin Miles Stoudenmire)

13:30-14:15	Zi Yang Meng, *Institute of Physics, Chinese Academy of Sciences*
	Self-learning Monte Carlo Method
14:15-15:00	Yang Wei Koh Patrick, Home researcher (physics), Singapore
	Low-lying excitations of quantum spin-glasses
15:00-15:10	📷 **Photo**
15:10-15:30	☕ **Break**

Session 3 (Chair: Yang Wei Koh Patrick)

15:30-16:15	Masato Okada, *The University of Tokyo and National Institute for Materials Science*
	Sparse modeling in condensed matter physics
16:15-17:00	Aurélien Decelle, *LRI, University of Paris-Sud*
	Ising inverse problem : recovering the topology of the network
17:00-17:45	Mikiya Fujii, *The University of Tokyo*
	Charge separation pathway via highly excited electronic states in organic photovoltaics
17:45-19:30	🍴☕ **Poster Session**

Program

Session 4 (Chair: Aurélien Decelle)

09:10- 09:55	Hiroshi Fujisaki, *Nippon Medical School* **Ab initio molecular tier model for quantum vibrational dynamics**
09:55- 10:40	Bing Huang, *University of Basel* **More efficient representations of compounds for machine learning models**
10:40- 11:25	Hieu Chi Dam, *Japan Advanced Institute of Science and Technology* **Design, select, and learning descriptors for materials informatics**
11:25-13:00	🍴 **Lunch**

Session 5 (Chair: Jascha Sohl-Dickstein)

13:00- 13:45	Ryo Tamura, *National Institute for Materials Science* **Estimation of effective models by machine learning**
13:45- 14:30	John Parkhill, *University of Notre Dame* **Neural Network Model Chemistries**
14:30- 15:15	Juan Felipe Carrasquilla, *D-Wave Systems* **Machine learning phases of matter**
15:15- 15:25	Takahito Nakajima, *RIKEN AICS* **Closing Remarks**

Deep Unsupervised Learning using Nonequilibrium Thermodynamics

Jascha Sohl-Dickstein
Brain team, Google

I will present a method for building probabilistic models of complex data-sets which is highly flexible, yet for which learning, sampling, inference, and evaluation are still analytically or computationally tractable. The essential idea, inspired by non-equilibrium statistical physics, is to systematically and slowly destroy the structure in a data distribution through an iterative forward diffusion process. We then train a reverse diffusion process to restore that structure, yielding a generative model of the data. By using a deep network to define the diffusion process, we are able to rapidly learn, sample from, and evaluate probabilities in deep generative models with thousands of layers or time steps. I will demonstrate the effectiveness of this model on several natural image datasets. I will also briefly discuss several other projects applying ideas from nonequilibrium statistical mechanics to training, sampling from, and predicting properties of machine learning models.

[1] Sohl-Dickstein J, Weiss EA, Maheswaranathan N, Ganguli S. Deep unsupervised learning using nonequilibrium thermodynamics. International Conference on Machine Learning. 2015. http://arxiv.org/abs/1503.03585

Machine Learning with Quantum-Inspired Tensor Networks

Edwin Miles Stoudenmire
University of California, Irvine

There is intense interest in the field of machine learning currently due to rapid algorithmic improvements, with many exciting applications including basic physics research. But popular machine learning techniques have drawbacks similar to ad-hoc variational wavefunction methods. Tensor networks could overcome these limitations just as in physics.

I will show how tensor networks fit naturally into the framework of non-linear kernel learning, where the key challenge is working in a high-dimensional vector space. Using a matrix product state ansatz, one can use DMRG type algorithms for optimization and realize benefits such as better scaling with training set size and automatic pruning of unnecessary parameters. I will conclude by highlighting interesting directions for future research such as interpretability and generalization.

Computational study on ultrafast electronic relaxation in an iron(II) complex

IUCHI, Satoru

Graduate School of Information Science, Nagoya University

Light-induced spin crossover of $[Fe(bpy)_3]^{2+}$ (bpy=2,2'-bipyridine) has been investigated by using ultrafast spectroscopies [1]. Understanding such a spin crossover process may provide useful insight into potential applications of new information technology and the dye-sensitized solar cells using iron(II) complexes. However, the detailed mechanisms of ultrafast relaxation in $[Fe(bpy)_3]^{2+}$ have not been well clarified.

By considering this current state of affairs, we have been developing a simple model electronic Hamiltonian for the d-d states of $[Fe(bpy)_3]^{2+}$ to perform molecular dynamics (MD) simulations for excited states [2]. It has been recognized that high level *ab initio* calculations are often necessary to accurately describe excited states of transition metal complexes, and thus on-the-fly MD simulations would be computationally too demanding. Therefore, although the information from such a simplified model Hamiltonian may not be quantitatively accurate, it would be still meaningful to obtain qualitative information about relaxation dynamics from simulations using the model Hamiltonian. In this talk, the basic idea of this model electronic Hamiltonian and some MD simulation results for understanding the ultrafast relaxation processes in $[Fe(bpy)_3]^{2+}$ will be presented.

[1] For example, W. Zhang *et al.*, Nature, **509**, 345 (2014); G. Auböck and M. Chergui, Nat. Chem., **7**, 629 (2015).

[2] S. Iuchi, J. Chem. Phys., **136**, 064519 (2012); S. Iuchi and N. Koga, ibid, **140**, 024309 (2014); S. Iuchi and N. Koga, Phys. Chem. Chem. Phys., **18**, 4789 (2016).

Self-learning Monte Carlo Method

Zi Yang Meng

Institute of Physics, Chinese Academy of Sciences

Self-learning Monte Carlo method [arXiv:1610.03137, 1611.09364] is a powerful general-purpose numerical method recently introduced to simulate many-body systems. In this work, we implement this method in the framework of determinantal quantum Monte Carlo simulation of interacting fermion systems. Guided by a self-learned bosonic effective action, our method uses a cumulative update [arXiv:1611.09364] algorithm to sample auxiliary field configurations quickly and efficiently. We demonstrate that self-learning determinantal Monte Carlo method can reduce the auto-correlation time to as short as one near a critical point, leading to O(N)-fold speedup. This enables to simulate interacting fermion system on a 100×100 lattice for the first time, and obtain critical exponents with high accuracy.

[1] J. Liu, Y. Qi, Z. Y. Meng and L. Fu, arXiv:1610.03137.
[2] J. Liu, H. Shen, Y. Qi, Z. Y. Meng and L. Fu, arXiv:1611.09364.
[3] X. Y. Xu, Y. Qi, J. Liu, L. Fu and Z. Y. Meng, arXiv:1612.03804.

Low-lying excitations of quantum spin-glasses

Koh Yang Wei

Home researcher

Recent numerical studies of quantum spin-glasses are usually performed by diagonalizing the full Hamiltonian using Lanczos algorithm [1] or by quantum Monte-Carlo simulations [2]. In this talk, we propose another approach inspired by theoretical chemistry called Configuration Interaction [3]. In this approach, one first solves for a Hartree-Fock ground-state which is simply a product of individual spin states. Using this Hartree-Fock state as a kind of `polarizable' vacuum state, a Hilbert space basis can be generated by exciting the spins of the vacuum state. When restricted to low-lying one and two-spin excitations, a partial basis can be constructed whose dimension scales quadratically instead of exponentially with the system size. Configuration Interaction allows us to simulate much larger systems sizes and at the same time going beyond the mean-field approximation. With this approach, we computed two quantities of interest due to recent advances in quantum annealing, the ground-state energy and the energy gap. Lastly, we discuss the possibility of solving optimization problems `semiclassically' using the Hartree-Fock energy, as opposed to the fully quantum mechanical quantum annealing.

[1] T. Jörg, F. Krzakala, J. Kurchan, and A.C. Maggs, Phys. Rev. Lett. **101**, 147204 (2008).

[2] A.P. Young, S. Knysh, and V.N. Smelyanskiy, Phys. Rev. Lett. **101**, 170503 (2008).

[3] Y. W. Koh, Phys. Rev. B **93**, 134202 (2016).

Sparse modeling in condensed matter physics
Masato Okada
The University of Tokyo and NIMS MI2I

The basic notions of sparse modeling (SpM) are as follows. First, high-dimensional data are assumed to have a sparse representation. Second, the number of explanatory variables should be reduced without loss of accuracy. Finally, explanatory variables are selected objectively, and effective models of target phenomena are constructed automatically [1]. In this talk, I explain why an SpM algorithm called LASSO works well, and give two applications of LASSO in condensed matter physics. The first example is an application of SpM to quasi-particle interference (QPI) experiment with scanning tunneling microscopy/spectroscopy (STM/STS) [2]. We showed that SpM improves efficiency and saves measurement time. The other is an application of Sparsity-promoting Dynamic Mode Decomposition (SpDMD) to coherent-phonon analysis [3]. We showed that SpDMD distinguishes signals of interest from the artifact noise of measurement system. Finally, I describe my future perspective of the data driven approach based on the SpM and the Bayesian inference in condensed matter physics [1].

[1] Y. Igarashi, K. Nagata, T. Kuwatani, T. Omori, Y. Nakanishi-Ohno, and M. Okada, J. Phys. Conf. Ser., 699(1), 012001 (2016).
[2] Y. Nakanishi-Ohno, M. Haze, Y. Yoshida, K. Hukushima, Y. Hasegawa and M. Okada, J. Phys. Soc. Jpn. 85, 093702 (2016).
[3] I. Akai, S. Murata, S. Aihara, S. Tokuda, K. Iwamitsu, and M. Okada, "Mode-decomposition analysis by SpDMD for coherent phonon signals (I)", 2016 Autumn Meeting of The Physical Society of Japan, 14pAL-3 (2016).

Ising inverse problem : recovering the topology of the network

Aurélien Decelle

LRI, University of Paris-Sud

During the past years, inverse problems have concentrated the attention of many different fields. In physics for instance, many works dealed with the possibility of inferring the coupling constants of statistical systems with many variables/particles. In compute science it is at the heart of machine learning, inferring the weights of neural networks that are then applied to recognition task, and we could mention many other applications in biology, social science, etc. In this presentation, I will focus on the particular task of inferring the interactions of an Ising model. The Ising model is particularly appealing for being a generative/probabilistic model. Therefore a good learning procedure will give us the interaction constants but also let us generate new configurations according to the inferred distribution. For this problem, I will show that our method, based on an approximation of the likelihood and a decimation procedure, is able to both infer the couplings and recover the topology (exactly or approximately depending on the difficulty) of the model in an automated way. I will then explain how it is possible to detect additional many-body interactions from the data.

Charge separation pathway via highly excited electronic states in organic photovoltaics

Fujii Mikiya[1,2,3]

[1]Department of Chemical System Engineering, School of Engineering, The University of Tokyo, Tokyo 113-8656, Japan
[2]JST, CREST, Tokyo 113-8656, Japan
[3]Elements Strategy Initiative for Catalysts & Batteries (ESICB), The University of Tokyo, Tokyo 113-8656, Japan

Dissociation of an electron and hole pair against the Coulomb interaction has been key mechanism in organic photovoltaics. However, the fine understanding has not been revealed yet. Some studies emphasize ultrafast charge separation called as "Hot" process[1] and while others have historically proposed "Cool" process[2] such as Marcus theory and Braun-Onsager theory. In addition to these controversial concepts, entropic diffusion is also stressed for the charge separation[3].

Here, we analysed the charge dissociation at atomic interface model that was constructed by molecular dynamics simulations. At first, we theoretically exhibit a threshold of separation distance in realistic bulk heterojunctions. Namely, the electron and hole can separate by entropic diffusion after the separation distance reaches to the threshold. Then, we theoretically showed explicit energy profiles for dynamical charge separations to reach the threshold and revealed that "Cool" process was hard to occur because the "Cool" process needs larger dissociation energy than the thermal fluctuation energy. Actually, the majority of free charges was experimentally revealed to be generated via "Hot" process. Finally, theoretical comparison of bilayer interface with intermix interface revealed miscibility dependences of the charge dissociation.

References

1. G. Grancini, et.al., Nat. Mat. 2012, 12, 29.
2. K. Vandewal, et.al., Nat. Mat. 2014, 13, 63.
3. B. A. Gregg, J. Phys. Chem. Lett. 2011, 2, 3013,

Ab initio molecular tier model for quantum vibrational dynamics

Hiroshi FUJISAKI

Department of Physics, Nippon Medical School

Molecular vibrations are important because they imprint the information of molecular configurations and its dynamical nature can be observed with recent advance of short-pulse (femtosecond) laser and time-resolved nonlinear spectroscopy. However, its theoretical understanding is still immature because it is an essential many body problem of quantum mechanical systems. Though the computer power has been increasing, there are huge obstacles for calculating quantum dynamics and potential energy surfaces (PESs). This is why we need to invoke some approximations and we here pursue an approximate method using the molecular tier model first introduced by Hynes and coworkers [1]. The tier model is an economical description of state space for quantum systems, and it starts from a parent node following daughter nodes with some connections. Each node represent a many-body quantum state and the connections between them are induced by anharmonicity of the molecular system considered. The state space is finally described as a branching tree structure and the total number of states can be minimized. Previous studies using the tier model often employed model PESs, but we here employ an *ab initio* PES with normal mode representation and quartic force field [2]. We try to apply this method to a recent experiment conducted by Rubtsov and coworkers [3], and compare the computational and experimental results by calculating the normal mode energies and kinetic energy for each atom, and analyze the classical aspects of the result using classical dynamics calculation.

[1] E.L. Sibert III, W. Reinhardt, J. Hynes, J. Chem. Phys. **81** (1984) 1115.

[2] H. Fujisaki, K. Yagi, H. Kikuchi, T. Takami, G. Stock, Chem. Phys. **482**, (2017) 86.

[3] V. Kasyanenko, S. Tesar, G. Rubtsov, A. Burin, I. Rubtsov, J. Phys. Chem. B **115** (2011) 11063.

MORE EFFICIENT REPRESENTATIONS OF COMPOUNDS FOR MACHINE LEARNING MODELS

Bing Huang and O. Anatole von Lilienfeld

Institute of Physical Chemistry and National Center for Computational Design and Discovery of Novel Materials, Department of Chemistry, University of Basel, Switzerland.

Over the last few years we have seen many great applications of machine learning (ML) models in the fields of chemistry and materials science. One of the major factors controlling the accuracy of ML models is the choice of representation of compounds. Numerous efforts have been devoted to develop more efficient representations, but systematic approaches seem to be absent. In this talk, I will talk about the representations developed by us and other groups using four associated categories: 1) continuous/discrete representations; 2) wave-function or charge density/energy-based representations (the former is based on Schrödinger equation directly, while the latter lays its foundation on the many-body expansion of energies); 3) non-alchemical/alchemical representations; 4) local/global representations. I will address several fundamentally important yet open questions regarding this topic: 1) what's a good representation in the first place (instead of its performance)? 2) why does one representation work better/worse than the other? 3) how could we design more and more efficient representations with systematically improved performance? 4) what's a formal definition of chemical compound space (CCS) in which all compounds reside in? Finally, I will briefly talk about another issue of paramount importance in this field, the strategy for selecting training set.

Design, select, and learning descriptors for materials informatics

DAM Hieu-Chi, PHAM Tien-Lam

Japan Advanced Institute of Science and Technology

One of the main mission in materials informatics is to discover knowledge from materials science data. The advanced data mining and machine learning methods are expected to fulfill this mission. However, the biggest difficulty in the process of applying data mining and machine learning techniques came from the development of materials descriptors.

In this talk, we will introduce our experiences in designing, selecting, and learning descriptors for materials. We demonstrate that knowledges of chemical physics on a materials system can be automatically extracted from experimental and first-principles calculated data represented by using these descriptors with integration of unsupervised and supervised learning techniques; these knowledges can be used to deepen the insight of the material system, improve empirical computational material science, and support the process of material design.

[1] Hieu-Chi Dam, Tu-Bao Ho, Ayumu Sugiyama, IJCAI 2011: 2424-2429 (2011).

[2] Hieu-Chi Dam, Tien-Lam Pham, Tu-Bao Ho1, Anh-Tuan Nguyen, and Viet-Cuong Nguyen, J. Chem. Phys. 140, 044101 (2014).

[3] Tien-Lam Pham, Hieu-Chi Dam, et al., J. Chem. Phys. 145 (15), 154103 (2016).

Estimation of effective models by machine learning

Tamura Ryo[1] and Hukushima Koji[1,2]

NIMS[1], U. Tokyo[2]

We develop a method for estimating the effective model from a given physical quantity by the machine learning based on the Bayesian statistics. In the estimation method, plausible model parameters that explain the given physical quantity are determined by maximizing the posterior distribution. We suppose that, with the help of machine learning technique based on a sparse prior and cross validation, relevant terms are successfully selected from a candidate model Hamiltonian including redundant terms [1]. The efficiency of the estimation method was tested by using synthetic magnetization curve data obtained by the classical Heisenberg model. Our results show that the proposed method enables estimation of the model parameters in the spin Hamiltonian correctly. It should be emphasized that the framework of our estimation method can be used not only for magnetization curves but also for any measured data as the input data. In addition, in the talk, it will be scheduled to discuss the Bayesian optimization for the effective model estimation which reduces computational time considerably [2].

[1] R. Tamura and K. Hukushima, Phys. Rev. B **95**, 064407 (2017).

[2] R. Tamura and K. Hukushima, in preparation.

Neural Network Model Chemistries

Parkhill John

The University of Notre Dame du Lac

Neural networks are being used to make new types of empirical chemical models as inexpensive as force fields, but with accuracy close to the *ab-initio* methods used to build them. I will present several applications of our open source suite for producing Neural Network Model chemistries; beginning with a discussion of NN's used to produce Orbital-Free Kinetic energy functionals[1]. I will also discuss new work, which studies various choices of energy decomposition and chemical embedding, and how these decompositions affect the accuracy and generality of the models produced.

Besides modeling potential energy surfaces, neural-nets can provide qualitative insights and make qualitative chemical trends quantitatively predictable. In this work we present a neural-network that predicts the energies of molecules as a sum of bond energies. The network learns the total energies of the popular GDB9 dataset to a competitive MAE of 0.94 kcal/mol. The method is naturally linearly scaling, and applicable to molecules of nanoscopic size. More importantly it gives chemical insight into the relative strengths of bonds as a function of their molecular environment, despite only being trained on total energy information. We show that the network makes predictions of relative bond strengths in good agreement with measured trends and human predictions. We show that DIM-NN learns the same heuristic trends in relative bond strength developed by expert synthetic chemists, and ab-initio bond order measures such as NBO analysis.

[1] Yao, K.; Parkhill, J. Kinetic Energy of Hydrocarbons as a Function of Electron Density and Convolutional Neural Networks. Journal of Chemical Theory and Computation 2016, 12, 1139-1147

[2] Yao, K.; Herr, J.; Parkhill, J. The Journal of Chemical Physics 146, 014106 (2017)

Machine learning phases of matter

Juan Felipe Carrasquilla

D-Wave Systems

I will discuss how neural networks can be used to identify phases and phase transitions in condensed matter systems via supervised learning. We show that standard feed-forward neural networks can be trained to detect multiple types of order parameter directly from raw state configurations sampled with Monte Carlo. In addition, they can detect highly non-trivial states such as Coulomb phases, and if modified to a convolutional neural network, topological phases with no conventional order parameter.

We show that this classification occurs within the neural network without knowledge of the Hamiltonian or even the general locality of interactions. Lastly, I will discuss the application of these ideas to fermionic systems exhibiting ordered, disordered and Anderson localized phases.

POSTER PRESENTATIONS

2nd Kobe Workshop （ 3 / 22 - 25, 2017 ）

Sasagawa Yoshinori（笹川 佳則）神戸大学(Kobe Univ.)（3/23, 24）

TEBD を用いた+−J ランダムイジングモデルのエンタングルメント・エントロピー解析

Analysis of Entanglement Entropy of the +−J Ising model using TEBD

Kenta Kanamori（金森 研太）名古屋工業大学（3/23）

固体内イオン伝導キャリアの低エネルギー領域同定の為の選択的サンプリング手法の開発

Kosuke Nakano（中野 晃佑）旭硝子 先端技術研究所（3/23）

第一原理計算と機械学習を利用した、無機材料の光学物性予測

Tomohiro Yonezu（米津 智弘）名古屋工業大学（3/23）

マルチタスクガウス過程によるコスト考慮型粒界構造探索

Unpei Nagashima（長嶋 雲兵）計算科学振興財団 FOCUS (3/23, 24)

Molecular mining by highly accurate molecular property estimation using a Supercomputer Aided Molecular Design with a Deep Learning on a Big Data and an AI technique.

Motomichi Tashio（田代 基慶）東洋大学（3/23）

PCBM/PCPDTBT 界面における電荷分離・再結合過程の
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A Single Reference Coupled Cluster Theory with Iterative Triple Excitation

for Ground State and Associated Equation of Motion Formulation for the Excited / Ionized State

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Quantum phase transition of frustrated triangle lattice Ising model coupled to a fermi surface

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Characterization of non-adiabatic electron wave packets in densely quasi-degenerate excited states

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Universal quantum criticality in two-dimensional interacting Dirac electrons

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時間依存 DMRG 法と量子アニーリング

Time dependent DMRG method and its application to quantum annealing

Shirakawa Tomonori（白川 知功）理化学研究所(RIKEN) （3/23, 24）

Local multiplets around the single vacancy in graphene

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MXenes: promising platforms for fundamental research and device application

Ahmad Ranjbar 理化学研究所(RIKEN) （3/24）

Structural, electronic and magnetic properties of Cr2AX（A= Al, Ge, Ga: and X=C, N, B）MAX phases

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Analysis of entanglement entropy of $\pm J$ Ising model using TEBD

Yoshinori Sasagawa[A], Hiroshi Ueda[B], and Tomotoshi Nishino[A]

Kobe University[A], RIKEN AICS[B]

Edwards-Anderson model [1], which is an Ising model for discussing the spin glass phase, has been the subject of numerous studies over many years. The Hamiltonian is $\mathcal{H} = -\sum_{ij} J_{ij}\sigma_i\sigma_j$ where σ_i takes the values ± 1. The nearest-neighbor couplings J_{ij} are independent random variables. For the $\pm J$ Ising model, J_{ij} takes $+J$ with probability p and takes $-J$ with probability $1-p$. The phase diagram of the 2-dimensional $\pm J$ Ising model is sketched in Figure 1. The dashed curve is Nishimori line[2]. The internal energy has a simple analytic expression and several exact results have been derived along the line.

In this research, we investigate whether it is possible to detect the phase boundary on Nishimori line using the entanglement entropy. This entropy is introduced to $\pm J$ Ising model through the quantum-classical correspondence. Let us consider a strip of the 2-dimensional $\pm J$ Ising model of the width N sites with free boundary conditions. The transfer matrix $\mathbf{T}^{(1)}$ including the bond randomness is applied to the boundary state $\mathbf{\Psi}^{(1)}$ to generate the next state $\mathbf{\Psi}^{(2)}$. The entanglement entropy is defined as $S = -\sum_i (\lambda_i)^2 \log(\lambda_i)^2$ where λ_i is singular values of $\mathbf{\Psi}^{(2)}$. We estimate S in each $\mathbf{\Psi}^{(n)}$ and use the average of S for the analysis.

The numerical calculation is operated by means of time evolving block decimation (TEBD)[3] method. Our result is Figure 2. It is confirmed that the entanglement entropy shows a peak structure around a critical temperature. The critical temperature is estimated at 0.959(1) by a finite size scaling method in agreement with the previous work[4].
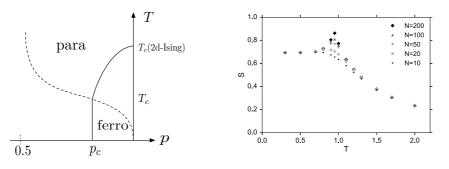

Figure 1: Phase diagram of $\pm$ J Ising model.

Figure 2: Entanglement Entropy S with respect to the temperature T.

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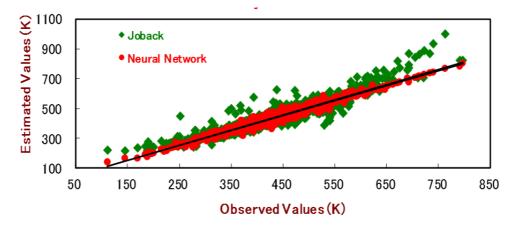
Molecular mining by highly accurate molecular property estimation using a Supercomputer Aided Molecular Design with a Deep Learning on a Big Data and an AI technique.

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Tyuoku, Kobe, 650-0047 Hyogo, Japan.

We have developed a novel property estimation equation with the group contribution scheme for molecular properties: boiling points, in the standard condition using a three layers perceptron type neural network

For deep learning, 1727 groups are newly defined as a set to reproduce the difference of isomers and to realize more reliable prediction than usual methods. 765 data of molecular boiling point are selected for education of the neural network. 953 data were applied to evaluate the efficiency of the equation.

The correlation of observed and predicted molecular boiling points by this work is better than the values by the classical technique as shown in Figure. The equation is applicable to estimate wide thermal range, namely high and low temperature region. Furthermore, the equation well reproduces the difference of boiling points for not only ortho-, meta-, and para- isomers but also cis- and trans-isomers.

Figure the correlation of observed and predicted molecular boiling points

Adiabatic electronic motion in forming covalent bond

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To explore the mechanism of chemical reactions, it is vital to examine the electronic motion in molecules. To this end, there have been many extensive theoretical studies of electronic motion. Among these, the study of electronic current density should be a useful approach in examining the time-evolving electronic motion. Defining an electronic wavefunction ψ, the electronic current density within quantum mechanics is expressed by

$$\mathbf{j} = \frac{1}{2i}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right). \tag{1}$$

However, when calculated within the Born-Oppenheimer approximation, as is useful for quantum and mixed quantum-classical dynamics, there holds $\mathbf{j} = \mathbf{0}$ because of the real-valuedness of the electronic wavefunction [1, 2]. Although some ways to solve this problem have been suggested [1, 2, 3, 4], how to describe the electronic current density is still open to improvement within the mixed quantum-classical theory.

In our study, in order to describe the electronic current density within the Born-Oppenheimer molecular dynamics, we introduce Maxwell's displacement current density to extract the current density related to bonding formation, which we call the electronic sharing current density. In the poster presentation, we apply this quantity to the covalent bonding formation in the H_2 system and thus, show the usefulness of this electronic sharing current density and reveal the reaction mechanism of the covalent bonding formation of the H_2 molecule.
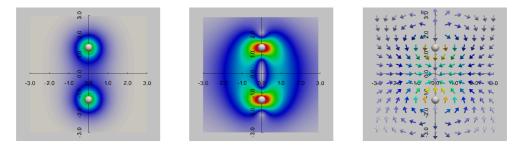

Figure 1: Electronic density (left panel), the absolute value of electronic current density (central panel) and electronic current density (right panel).

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[4] V. Pohl and J. C. Tremblay, Phy. Rev. A. **93**, 012504 (2016).

Theoretical study on hot charge transfer state and dimensional effect for organic photocell device

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Organic photocells using π-conjugated oligomers and polymers have been gathering much attention as one of renewable natural power resources. The manufacturing of organic semiconductors does not need high-temperature processes unlike inorganic semiconductors. Low-temperature processes help to reduce the production costs of organic photocells. In addition, the unique features of organic semiconductors, such as versatility of functionalization, thin film flexibility, and easy processing, are attractive to create devices. However, at present the conversion efficiency of organic photocells remains lower compared with inorganic photocells. In order to improve the efficiency, the mechanisms of photocurrent generation in organic semiconductors have been actively investigated. The dissociation of electron-hole pair (exciton) generated by adsorbed photon energy is a key process.

We theoretically investigate the exciton dissociation process through hot states at the donor-acceptor interface of organic photocells. We expanded the formalism of Rubel et al. (*Phys. Rev. Lett.*, **100**, 196602, 2008.), and adopted the theoretical concept of Arkihov et al. (*Phys. Rev. Lett*., **82**, 1321, 1999.) to consider hot charge transfer (CT) states. The hot CT state effect is effective to raise the probability to separate electron-hole pair. We also found that cooperative behaviors between the hot CT state and the dimensional effects are essential for efficient exciton dissociations. In the workshop, we will discuss the details of our theoretical study for organic photocells.

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Group Molecular Orbital Method For Large Molecular Systems

Tomomi Shimazaki(RIKEN,AICS), Kazuo Kitaura(RIKEN,AICS),
Dmitri G. Fedorov(AIST,CD-FMat), Takahito Nakajima(RIKEN,AICS)

An algorithm to solve the Huzinaga subsystem self-consistent field equations[1] is proposed using two approximations: a local expansion of subsystem molecular orbitals and a truncation of the projection operator. Test calculations are performed on water and ammonia clusters, and n-alkane and poly-glycine. The errors were 2.2 and -0.6 kcal/mol for $(H_2O)_{40}$ and $C_{40}H_{82}$, respectively, at the Hartree-Fock level with the 6-31G basis set.

[1] S. Huzinaga and A. A. Cantu, J. Chem. Phys. **55**, 5543 (1971).

Fast evaluations of two-electron repulsive integrals using pseudospectral methods

Keisuke Sawada

RIKEN Advanced Institute for Computational Science

A fast estimation of two-electron repulsive integrals (ERIs) is an important and imperative subject in any *ab-initio* quantum chemical calculations. Since the computational cost of the ERIs formally increases as N^4, where N is the number of basis functions, we often suffer from much time-consuming estimations in large molecular systems.

In order to address the tough problem, several methodologies have been developed to date. Among them, the pseudospectral (PS) method is a strong candidate for a quick and efficient evaluation of the ERIs. In the PS method, one analytical integral is replaced by a numerical summation consisting of discrete grid points and the computational cost is reduced from $O(N^4)$ to $O(MN^2)$, where M is the number of grid points. Because of the discretization of a continuous integral space, the PS method is not only a fast method for estimations of the ERIs but also suitable for recent massively parallel computations using numerous CPU cores.

In this study, we implement the PS and PS-GAP methods into NTChem program and investigate the performances of these methods using the Flat-MPI and MPI/OpenMP hybrid parallelized codes. The PS-GAP method is further accelerated method that the PS and Gaussian-and-plane-wave (GAPW) methods are combined. In large molecular system which includes more than 8,000 basis sets, we find that the PS and PS-GAP methods show a good scaling with respect to used CPU cores and become much faster than the analytic integral methods. Moreover, the PS-GAP method exhibits the low-dimensional scaling in terms of the number of basis sets and achieve less than $O(N^2)$ computational costs.

Large Scale Matrix Polynomial Computation
for Linear Scaling Quantum Chemistry

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Self-consistent field cycles in quantum chemistry calculations usually require computing the eigendecomposition of a matrix, an approach that has been aided by the development of large scale eigenvalue libraries. However, the cubic scaling cost associated with computing the eigendecomposition has become a bottleneck as researchers try and investigate larger and larger systems. In the case where the operator can be represented as a sparse matrix, however, there exist methods for computing the density matrix in linear time. In particular, methods based on matrix polynomials have been shown to efficiently approximation the matrix functions used in linear-scaling quantum chemistry. Recently, our group has begun development of a highly parallel library for computing polynomials of sparse matrices on the K computer. This library will be able to accelerate quantum chemistry calculations across a number of different codes. In this session, I will present the parallel algorithms at the basis of this library, and our current progress and insights.

A Single Reference Coupled Cluster Theory with Iterative Triple Excitation for Ground State and Associated Equation of Motion Formulation for the Excited / Ionized State

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[1] Computational Molecular Science Research Team,
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[2] VINAS Co. Ltd.

In this poster, I shall present our recent efforts towards development of a single reference coupled cluster theory which is capable of including the effect of connected triple and higher excitations in an iterative manner within singles and doubles framework. The most salient feature of our formulation is that the computational cost increases only marginally than the traditional Coupled Cluster Singles and Doubles. I shall also present the corresponding Equation of Motion (EOM) formalism for accurately predicting the excitation and ionization energies. Some preliminary numerical examples of our formalism will be presented and our results will be compared and contrasted to other variants of traditional single reference theory.

[1] Y. Akinaga and T. Nakajima, J. Phys. Chem. A, 2017, 121(4), pp.827-835

Characterization of non-adiabatic electron wave packets in densely quasi-degenerate excited states

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The present study of characterizing non-adiabatic electron wave packet dynamics in a highly quasi-degenerate excited electronic states is intended to explore and design a new chemical functionality by using a superposition of electronic excited states created by external laser fields and molecular environment. Inspired by the remarkable advances in the experimental measurements of ultrafast dynamics including electron dynamics in molecules [1,2], we have developed a theory of non-adiabatic electron wave packet dynamics as a tool to achieve the goal [3,4].

We demonstrate following five types of characterization of complex excited electron wave packet [3,4,5,6] with use of

(a) electronic state density [3]

(b) unpaired electron, bond order spatial distribution and current [3,4,5,6]

(c) two electron correlation of unpaired electron [3]

(d) state diffusion dynamics [3]

(e) reactivity depending on laser polarization. [4]

Necessities of characterization of electron wave packet are discussed with related to a possibility of a novel chemical reaction field induced in the boron cluster via external/internal state couplings.

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