International Workshop on Computational Science 2017
February 15–18, 2017
Kanazawa University, Japan

Date February 15–16, 2017 (Main Session)
February 17–18, 2017 (Special Session)

Venue Kanazawa University, Japan (Kakuma campus)
Kakuma-machi, Kanazawa 920-1192
Lecture hall: **203**, main building of Graduate school of natural science and technology, building S1.
http://www.kanazawa-u.ac.jp/e/campuses/

URL http://polaris.s.kanazawa-u.ac.jp/iwcs2017/

This workshop is supported by Kanazawa University SAKIGAKE Project.

The special session of IWCS2017: "Design of Novel Magnetic Materials for Device Applications: Simulation and Experiment" is co-organized by Post-K Priority Issue 7 - Creation of new functional devices and high-performance materials to support next-generation industries ("CDMSI")

Program of the Main Session

February 15

13:30 – 13:40 Opening

Invited lectures (25min + 5min Q&A)

13:40 – 14:10 Edy Tri Baskoro (Institut Teknologi Bandung)
Ramsey number for graphs

14:10 – 14:40 Mirza Satriawan (Universitas Gadjah Mada)
Multicomponent Dark Matter in the Mirror Model with Massive Mirror Photon

14:40 – 15:10 Jiraphan Suntornchost (Chulalongkorn University)
Variable selection for a regression model when dependent variable is subject to measurement errors

15:10 – 15:40 Kazutomo Kawaguchi (Kanazawa University)
Theoretical Study of Intermolecular Interactions for protein systems

15:40 – 16:00 Break

16:00 – 17:00 Short presentations (3min)

17:00 – 18:00 Poster session (room **202**)

February 16

Invited lectures (25min + 5min Q&A)

09:30 – 10:00 Acep Purqon (Institut Teknologi Bandung)
Urban Physics and Its Implementation in Predicting Economic Growth Related to High Speed Train Development

10:00 – 10:30 Manabu Oura (Kanazawa University)
Ring of the weight enumerators of d_n^+

10:30 – 11:00 Fatimah A. Noor (Institut Teknologi Bandung)
Modeling of Tunneling Current in High-k-based MOS Capacitors by Considering the Effects of Coupling between Longitudinal and Transverse Motions

11:00 – 11:20 Break

11:20 – 11:50 Suprijadi (Institut Teknologi Bandung)
Experimental and Computational study on physical properties based on granular system

11:50 – 12:20 Triati Dewi Kencana Wungu (Institut Teknologi Bandung)
Natural Clay Mineral as Adsorbent for Health and Environment Applications: A Density Functional Theory Study

12:20 – 12:50 Tatsuki Oda (Kanazawa University)
Research and development of high performance material for voltage torque MRAM by means of first-principles calculation

12:50 – 13:00 Closing

Program of the Special Session
"Design of Novel Magnetic Materials for Device Applications: Simulation and Experiment"

February 17

9:30 – 9:35	Opening
9:35 – 10:15	Y. Sakuraba (NIMS) *Exploration of ferromagnets with large anomalous Nernst effect for novel thermoelectric applications*
10:15 – 10:40	Y. P. Mizuta (Kanazawa Univ.) *Skyrmion-driven thermoelectric conversion: An ab intio study*
10:40 – 11:00	Break
11:00 – 1:40	T. Koretsune (RIKEN) *First-principles calculation of Dzyaloshinskii-Moriya interaction*
11:40 – 12:05	M. Ohashi (Kanazawa Univ.) *Superconductivity of chromium thin film*
12:05 – 13:35	Lunch
13:35 – 14:15	A. Kawasuso (QST) *Application of spin-polarized positron spectroscopy to some ferromagnetic systems*
14:15 – 14:55	K. Hyodo (JST-CREST, Tohoku Univ.) *First-principles study on intrinsic and extrinsic anomalous Hall conductivity of transition metal alloys*
14:55 – 15:20	Break
15:20 – 16:00	A. Edström (ETH Zürich) *Computational Design of Transition Metal Magnets with Large Magnetocrystalline Anisotropy*
16:00 – 16:40	T. Nozaki (Tohoku Univ.) *Voltage control of magnetization using magnetoelectric antiferromagnet Cr_2O_3 sputtered thin film*
16:40 – 17:05	M. Obata (Kanazawa Univ.) *Investigation of spin dependent van der Waals density functional approach*
17:45 –	Banquet (for special session participants, Sumire-Tei in Kanazawa university)

February 18

9:10 – 9:50 K. Ohishi (CROSS)
Chiral magnetism in $CsCuCl_3$ probed by polarized neutron scattering and muon spin rotation

9:50 – 10:30 H. Nakanishi (NIT, Akashi College)
Quantum simulation for the motion of positive-muon in materials and its application for Mu-SR spin state analysis

10:30 – 10:55 J. B. Lin (NIMS)
Linear-scaling DFT study on the structural optimization and electronic properties of real size Ge/Si core-shell nanowires

10:55 – 11:15 Break

11:15 – 11:55 Y. Onose (Univ.Tokyo)
Nonreciprocal propagation of elementary excitations in noncentrosymmetric magnets

11:55 – 12:35 Y. Ohnuma (JAEA)
Theory of spin current generation

12:35 – 12:40 Closing

List of posters

1. Yoshiho Akagawa (Kanazawa University)
   Numerical simulation for dynamical elastic contact problem

2. Saeful Akhyar (Kanazawa University)
   Smoothed particle hydrodynamic simulation of accretion disk in cataclysmic variable

3. Hasan Al Rasyid (Kanazawa University)
   First-Principles Study of Electronic, Magnetic, and Optical Properties of Nickel Cobaltite: DFT and QSGW methods

4. Fadil Habibi Danufane (Kanazawa University)
   Holonomic Gradient Method for the Distribution Function of the Largest Root of Complex Non-Central Wishart

5. Yosuke Funato (Kanazawa University)
   First-principles study on θ-phase in solid oxygen

6. Kouta Futai (Kanazawa University)
   Numerical study of an adaptive Lagrange-Galerkin scheme for pure convection problems

7. Nurul Ikhsan (Kanazawa University)
   Theoretical study on multi-functional Fe/MgO interface: investigation of perpendicular magnetic anisotropy origin

8. Tomosato Kanagawa (Kanazawa University)
   First principles calculation of magnetic anisotropy energy on double interfaces slab systems of X/Fe/MgO

9. Hiroyuki Kitano (Kanazawa University)
   Numerical simulation of contact problem of an elastic body with friction

10. Susumu Minami (Kanazawa University)
    Hyperfine structure of muonium in GaN

11. Masum Murshed (Kanazawa University + University of Rajshahi, Bangladesh)
    On the prediction of storm surge along the coast of Bangladesh

12. Takumi Nakano (Kanazawa University)
    3D simulation of crack propagation in an elastic body by a phase field model

13. Irma Palupi (Kanazawa University)
    An Implicit Boundary Integral Method for Laplace Problem

14. Riska Wahyu Romadhonia (Kanazawa University)
    Finite elements method of ergodic distribution function for Jaffe model

15. Ayu Shabrina (Kanazawa University)
    Numerical method of nonlinear Black Scholes equation for American options pricing

16. Shogen Shioda (Kanazawa University)
Computation of an inverse free boundary problem for a shape optimization method

17. Hiroki Yamamoto (Kanazawa University)
A gradient flow structure of the Maxwell-type viscoelastic model and its finite element analysis

18. Yamaoka Ryohei (Kanazawa University)
4 way-hexagonal symmetric crystalline method and 2 dimensional snow crystal model allowing collision / splitting

19. Takuro Yoneda (Kanazawa University)
Development of a finite element method for a delamination model and its simulation

20. Yang Zhenxing (Kanazawa University)
Minimum energy state and gradient flow for interaction energy of particles

RAMSEY NUMBER FOR GRAPHS

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Abstract. Ramsey theory first appeared in the context of propositional logic (1928). This theory became famous after Paul Erdos and George Szekeres (1935) applied it in graph theory. Determining the exact values of the classical Ramsey numbers R(m; n) has received a lot of attention. However, the results are still far from satisfactory. On the other hand, graph Ramsey theory as one of its generalizations has grown enormously in the last four decades to become presently one of the most active areas in Ramsey theory. For any graphs G and H, the Ramsey number $R(G,H)$ is denoted as the least integer t such that any red blue coloring on the edges of the complete graph on t vertices yields either a red G or a blue H as a subgraph. The Ramsey number $R(G,H)$ has been studied for various pairs of G and H. In this talk, we shall give a survey on the finding of Ramsey numbers $R(G,H)$ if one of G and H is a wheel. We also discuss the Ramsey numbers $R(G,H)$ if either G or H is a union of graphs.

Multicomponent Dark Matter in the Mirror Model with Massive Mirror Photon

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A modified mirror model, whose gauge group is $\mathrm{SU(3)}_1 \otimes \mathrm{SU(3)}_2 \otimes \mathrm{SU(2)}_L \otimes \mathrm{SU(2)}_R \otimes \mathrm{U(1)}_{Y1} \otimes \mathrm{U(1)}_{Y2}$ and the particles content consist of the ordinary SM particles (plus the right handed neutrinos) and their parity mirror partners, can provide a multicomponent dark matter sector, consist of cold and warm dark matter components. I add to the original mirror model a singlet scalar ϕ_e and its mirror partner ϕ_E, whose quantum numbers are the same as the singlet right handed electron and its mirror-partner. The ϕ_E can have a non zero VEV, while the ϕ_e remains with zero VEV. As consequences: Mirror photon will obtain mass whose order is around the neutral weak boson mass, rendering the mirror electromagnetic-like interaction to be weak; The ϕ_e will decay slowly producing more entropy in the ordinary sector, providing an escape to the BBN constraint for this model; There is a mixing among the ordinary and mirror neutrinos, and the singlet and doublet mirror electrons, as a result the mirror doublet electron have masses in the keV order, becoming the warm dark matter component of this model.

The asymmetric part of mirror baryons have energy density at the same order as Ω_B, and since the mirror electromagnetic-like interaction is weak, the mirror baryons can condense and become a very large mirror atomic-nucleus, becoming the cold dark matter component of the model. The symmetric part of mirror electrons cannot annihilate into mirror photons, and its abundance is comparable to the ordinary photons but suppressed by the temperature different of the two sectors. Since their mass is in the keV order, they can contribute an energy density in the same order as Ω_B.

PACS numbers: 12.60.-i, 11.30.Er, 95.35.+d

Variable selection for a regression model when dependent variable is subject to measurement errors*

Partha Lahiri and Jiraphan Suntornchost†

Abstract

In this paper, we first examine the accuracy of a given variable selection criterion (e.g., adjusted R^2) for a regression model when dependent variable is subject to measurement error variability. Such a situation occurs, for example, in small area estimation where one explores the relationship between the true small area mean and a set of known auxiliary variables. We show that the approximation error, that is, the difference between the standard variable selection criterion and the corresponding ideal variable selection criterion without any measurement error variability, does not converge to zero even for a large sample size. In our simulation, we notice that standard variable selection criterion could severely underestimate the ideal variable selection criterion in presence of high measurement error variability. We device a simple adjustment to the standard variable selection criterion that reduces the approximation errors considerably. In particular, we show that the approximation error for our new variable selection criterion converges to zero for large sample size. We demonstrate through simulation that our proposed variable selection criterion tracks the ideal variable selection criterion very well compared to the standard variable selection criterion.

Key Words: Adjusted R^2; small area estimation.

*The research was supported in part by National Science Foundation grant SES-0851001 and a National Institute of Health subcontract from the University of Michigan.

†Presenter

Theoretical Study of Intermolecular Interactions for protein systems

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Association of protein molecules plays a key role in many protein functions, such as signal transduction, transcription, and electron transport in photosynthesis. We have discussed the association of protein molecules by using coarse grained model in which protein-protein interaction is represented by only van der Waals interaction [1]. We have also investigated that the effective attraction interacts between a protein molecule and its ligand molecule in a water solvent by using all-atom molecular dynamics (AAMD) simulations [2].

In this study, we construct the coarse grained model to represent the effective interaction between protein molecules in a water solvent. The effective interaction between two amino acid side chains in a water solvent is calculated as a function of the distance between them by using AAMD simulations. The coarse grained potential function for each amino acid side chain is constructed to represent the effective interaction obtained by the AAMD simulations. We show that the Langevin dynamics simulation with Gō-like model and our coarse-grained model reproduces a homotetramer complex structure of GCN4-pLI and that the interactions between hydrophobic amino acid residues promote the association of GCN-pLI monomers [3].

[1] M. Rusmerryani, M. Takasu, K. Kawaguchi, H. Saito, H. Nagao, JPS Conf. Proc., 1 (2014) 012054.

[2] K. Kawaguchi, H. Saito, S. Okazaki, H. Nagao, Chem. Phys. Lett., 588 (2013) 226-230.

[3] K. Kawaguchi, S. Nakagawa, S. Kinoshita, M. Wada, H. Saito, H. Nagao, Mol. Phys. (2016) in print.

Urban Physics and Its Implementation in Predicting Economic Growth Related to High Speed Train Development

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Abstract. Contribution to complexity in urban problems and its challenges can be provided nowadays using urban physics, a well-established discipline, incorporating relevant branches of physics, environmental chemistry, aerodynamics, meteorology and statistics. Growth of cities and their connections are complex and very similar to organic systems in biology. Interventions in the terms of policy, that borrow principle from theoretical physics, could help to improve urban planning (Pollock, 2016). Pedestrian wind comfort, pedestrian thermal comfort, building energy demand, pollutant dispersion and wind-driven rain are five eminent problems in the field of urban physics, closely linked to urbanisation (Moonen et al., 2012). Using networks in analyzing available big data, e.g. urbanisation, economic growth, education level, population quality, etc., and correlating them might produce some interesting phenomena such as small world effect (Newman, 2008). Development of high seed train Jakarta-Bandung and related analysis to growth of cities along the paths is a hot current topic, since it requires by the government, especially the local ones, in supporting their strategy and policy to control the organic development of economics, which could trigger over population, social problem, and even crime rate, besides increasing the local income and speeding up land opening. It might potentially result in excessive resource utilization in the Jakarta Bandung region (Firman, 2009). In this talk influence of policy are discussed, how it can change utilization of region and cities passed by the train path.

References

1. Firman T 2009 Habitat Int. 33 327
2. Newman M 2008 Phys. Today 61 33
3. Moonen P, Defraeye T, Dorer V, Blocken B and Carmeliet J 2012 Front. Arch. Res. 1 197
4. Pollock K 2016 Nature 531 S64

Ring of the weight enumerators of d_n^+

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First we recall the connection among algebraic combinatorics, the invariant theory of the finite groups and the theory of modular forms. And then, we take up a special Type II code d_n^+. It is shown that the ring over $\mathbf{C}$ generated by the weight enumerators of d_n^+ is finitely generated over $\mathbf{C}$. Moreover, we can give enough elements to generate the ring. This result is applied to determine a set of generators of the ring for small genus.

Modeling of Tunneling Current in High-k-based MOS Capacitors by Considering the Effects of Coupling between Longitudinal and Transverse Motions

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Since sixty years ago, many theoretical and experimental investigations have been done to study electron tunneling processes in heterostructures. As one type of heterostructures, silicon-based metal-oxide-semiconductor field effect transistors (MOSFETs) are the base of modern computers and telecommunications, and the drudge of the integrated circuit technology. Because of emerging applications involving lower voltage operation, higher speed and density, MOSFETs are aggressively scaled down to the sub-micrometer regime and below and consequently the shrinking of the SiO_2 gate-dielectric thickness down to sub-nm region. Huge tunneling current occurs and power dissipation becomes significantly high when the SiO_2 gate-dielectric thickness is less than 1.5 nm. High dielectric constant (*k*) materials are the most potential dielectrics to substitute SiO_2. A gate oxide demanded to replace SiO_2 is a stack of SiO_2 and a high-*k* layer known as a high-*k* dielectric stack because an ultra thin interfacial SiO_2 often forms during the fabrication process. Several models have been proposed to calculate the tunneling current in high-*k* -based MOS capacitors. However, they did not consider a coupling effect between transverse and longitudinal energies and anisotropic masses. On the other hand, it is well known that an electron does not move in the longitudinal direction only but also in the transverse one. In this research, we develop a model of tunneling current in high-*k* -based MOS capacitors by taking into account the coupling effect of transverse-longitudinal motion and anisotropic masses. The calculated tunneling current is then compared to the measured one to examine the accuracy of the model.

Experimental and Computational study on physical properties based on granular system

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Abstract

In recent years, research on granular system computation increase significant in department of Physics ITB. The computation in many fields were applied with different methods such as smoothed particle hydrodynamics (SPH), moving particle semi-implicit (MPS), molecular dynamics (MD) and other standard methods. The other hand, to clarify the results, we did some experiments to refine the model. In this presentation, we will present experimental and computational study on fluid drop, Brazil-nuts effect phenomenon, and two dimensional (2D) material under uniaxial force.

We do simple experiment on fluid drop under on a filter like sheet to clarify the result on effect of particle size fluid drop and the possibility to separate two different fluids base on particle size. Research on Brazil-nut effect was begun more than 30 years ago, but still interesting because of the application of this phenomena can be implemented in many different area. The simple experiment and simulation based on granular system shows us the influence of frequency and amplitude. In the 2D material the model were based on experiment on thin rubber under uniaxial forces and atomic bond model, the results shows good relation between forces and elongation of rubber. Based on this results, we applied to silicine with its parameter and behavior for studying morphology changing during stressed under controlled forces. Also we studied on the the effect of morphology change to electronics properties of silicine using DFT by VASP.

Keywords :
granular, sph, mps, md, electronic behaviour

Natural Clay Mineral as Adsorbent for Health and Environment Applications: A Density Functional Theory Study

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Abstract

In this study, we present application of natural clay mineral, that is montmorillonite, using first principle-calculations by means of electronic structure calculation with emphasis on approaches based on Density Functional Theory (DFT). A montmorillonite has a large surface area which brings beneficial to adsorb any atoms or molecules to its surface. Therefore, montmorillonite can acts as a good adsorbent material and hence can be used for a wide variety of environmental and health applications. Here, the mechanism of atom/molecule adsorption on the surface of Montmorillonite is investigated to seek their interaction in an atomic scale point of view. The atoms such as Pd and Cs are used in this simulation to obtain the results of their interaction with Ca-montmorillonite. For the calculation method, we used DFT within Kohn-Sham formula implemented in Vienna *Ab initio* Simulation Packages (VASP). The generalized gradient approximation (GGA) within the Perdew–Burke–Ernzerhof (PBE) functional was employed for the exchange-correlation energy. The Brillouin zone was sampled using 5 x 5 x 1 Monkhorst-Pack k-point grid and the cut off energy is 520 eV. The total energies are converged to 0.01 meV.

Keywords: DFT, montmorillonite, Pd, Cs

Research and development of high performance material for voltage torque MRAM by means of first-principles calculation

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Since the electric-field (EF) control of ferromagnetism was discussed in 2000 [1], the study on EF effect in the thin magnetic film has been performed very actively. After the interface of Fe/MgO was proposed [2], much effort has been devoted in order to realize a spintronic device application. A proto-type of voltage torque magnetic random access memory (MRAM) was proposed as an ultra-low-power high-speed memory [3]. Its technique contains new voltage-controlled writing method for nonvolatile solid-state magnetic memory. Such memory is considered to have a potential for replacing the roles of conventional SRAM and DRAM. To build a spintronic device for widely used memory, various kinds of development are requested. Such development will be achieved in a part of the ImPACT (Impulsing PAradigm Change through disruptive Technologies Program) project, organized by CAO(Cabinet Office, government of Japan), managed by Masashi Sahashi in Tohoku University, and sponsored by JST(Japan Science and Technology agency). Kanazawa University (main researcher is Tatsuki Oda) has been contributed to the project since April in 2016 from the side of computational science.

In the project, Kanazawa group has studied both the analysis of mechanism and the material design for high performance interface magnetic anisotropy and voltage control. With using first-principles computations based on the density functional theory, we have investigated the electronic, atomic, and magnetic structures in the Fe/MgO interface and its family. Our approach employs the spin-orbit interaction which comes from the relativistic effect of electrons around atom nucleus, being enable to estimate the magnetic anisotropy energy (MAE) and the EF effect (EFE) imposed on the interface. In our simulation, the lattice constant in interface plane, the materials of ferromagnet and insulator, and the coordinates of atoms are treated as input parameters. Though both the analysis and simulation, the conditions for high performance system is desirable. I introduce the project and explain the approach based on computational science in the talk.

This work was supported by the ImPACT Program of Council for Science, Technology and Innovation (Cabinet Office, Japan Government) and by the Kanazawa University SAKIGAKE Project.

[1] H. Ohno *et al.*, Nature **408**, 944 (2000); Nat. Mater. **9**, 952 (2010).

[2] T. Maruyama *et al*., Nat. Nanotech. **4**, 158 (2009).

[3] Y. Shiota *et al*., Nat Mat. **11**, 39 (2012).

Exploration of ferromagnets having large anomalous Nernst effect for novel thermoelectric applications

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Anomalous Nernst effect (ANE) is a thermoelectric phenomenon that generates an electric voltage to the cross product direction between the magnetization and the temperature gradient in a ferromagnetic material. Previously, Sakuraba et al. proposed that there are advantages to apply ANE for thermoelectric applications owing to its three dimensionality in contrast to one dimensionality of conventional Seebeck effect, e.g. the electric voltage can be easily increased by making a simple laterally connected structure etc. (Fig.1) [1,2]. However, to improve thermoelectric power originating from ANE (S_{ANE}) is necessary to make practical applications more realistic. Since anomalous/spin Hall effect (AHE, SHE) and ANE are related phenomena, we can learn how to enhance ANE from previous studies on AHE and SHE. Niimi et al reported that the spin-Hall angle in Cu can be drastically enhanced by heavy elements Ir and Bi-doping.[3,4] Therefore, in this study, we have investigated the effect of heavy elements (Ta, Ir, Bi) doping to Fe film for an enhancement of ANE effect.

The heavy elements doped Fe films were deposited by a co-sputtering method using pure Fe and Ta/Ir/Bi targets on MgO substrates. ANE effect was measured by applying temperature gradient and external magnetic field to the in-plane and out-of-plane directions of the films, respectively.

It was found that AHE and ANE in Fe films were drastically enhanced by doping Ir. The Fe film with 16-18 at.% Ir shows about 4 times larger thermopower S_{ANE} and one order of magnitude larger ANE angle θ_{ANE} (defined in S_{ANE}/S_{SE} here) than those in pure Fe film (Fig.2). Observed θ_{ANE} of 38% is the highest ever reported in any ferromagnetic materials such as FePt ($\theta_{ANE} \sim 15\%$). Although S_{ANE} is still rather small due to small S_{SE} of Fe and the mechanism of the enhancement of S_{ANE} has not been clarified yet, the enlargement of θ_{ANE} by heavy element doping is S_{ANE} for further improvement of thermopower of ANE.

[1]Sakuraba et al., APEX 6, 033003 (2013), [2]Y. Sakuraba, Scripta Materialia 111, 29-32 (2016)., [3]Y. Niimi et al., Phys. Rev. Lett. 109, 1566

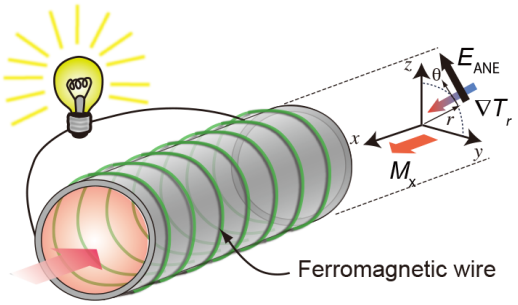

Figure 1: Example of thermoelectric power generation based on ANE using a tube shape heat source.[2]

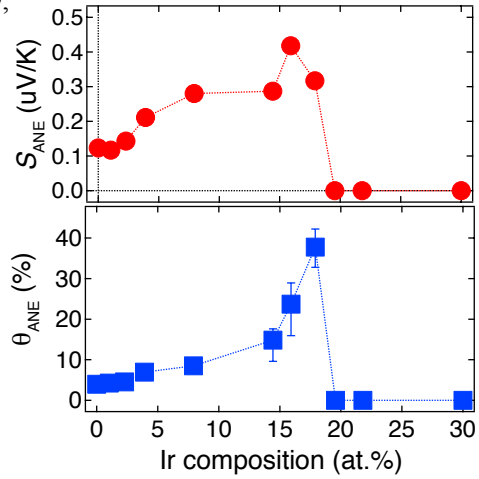

Figure 2: Ir composition dependence of thermopower of ANE (S_{ANE}) and anomalous Nernst angle (θ_{ANE}) in Ir-doped Fe films.

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Skyrmion-driven thermoelectric conversion: An *ab intio* study

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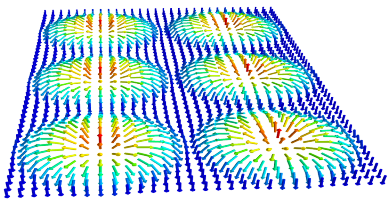
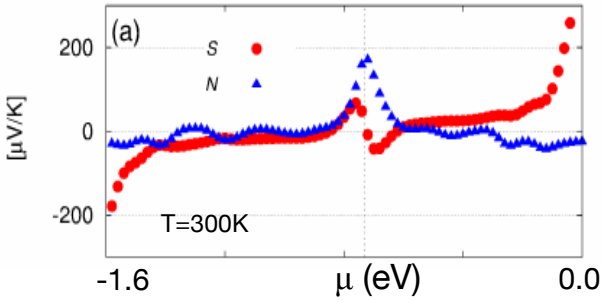
The magnetic skyrmion, a topological object formed by spins in condensed matter, exhibits many peculiar properties, among which we target the anomalous Nernst effect (ANE), heat-to-electricity conversion in transverse direction, driven by an emergent magnetic field ***B*** originating from its spin texture. We have found through *ab initio* calculations on a single *s*-orbital model using the codes *OpenMX* [1] and *Wannier90* [2] that, in the skyrmion crystal (SkX) phase (Fig.1), where skyrmions are crystallized in two dimensions, the crystal-momentum component of ***B*** generates large ANE when chemical potential μ is properly tuned (Fig.2) [3]. This was found to be due to rapid variation of Chern numbers with respect to energy in the band structure, which had been implied in an earlier tight-binding model analysis [4] and further studied *ab initio* [5]. Following such an observation in the simplest model of square SkX [3], our subsequent computations on more realistic models of transition-metal oxides also have predicted possible large ANE.

This motivates further studies in quest of better thermoelectric materials that exploit this effect.





Left: Fig. 1. An example of Skyrmion crystal

Right: Fig. 2. Large ANE coefficient (blue) in a SkX (*s*-orbital model of Ref. [3])

[1] T. Ozaki *et al.*, http://www.openmx-square.org.

[2] A.A. Mostofi *et al.*, http://www.wannier.org.

[3] Y. P. Mizuta and F. Ishii, Scientific Reports **6,** 28076 (2016).

[4] K. Hamamoto, M. Ezawa and N. Nagaosa, Phys. Rev. B **92**, 115417 (2015).

[5] H. Sawahata, Y. P. Mizuta and F. Ishii, International Workshop on nano-spin conversion science & quantum spin dynamics, Poster Q-22, Oct.14, 2016, Tokyo.

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First-principles calculation of Dzyaloshinskii-Moriya interaction

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In noncentrosymmetric magnetic systems, the spin-orbit coupling induces an antisymmetric exchange interaction between spins, called Dzyaloshinskii-Moriya (DM) interaction. This interaction favors twisted magnetic structures unlike the usual symmetric interactions. Thus, controlling this unique interaction opens a new possibility of engineering magnetic behavior. Here, we show two approaches to evaluate the DM interaction from first principles. One can be regarded as a perturbation with respect to the exchange couplings and the DM interaction is expressed by the off-diagonal spin susceptibility[1]. The other can be obtained by expanding the effective Hamiltonian with respect to the spatial derivative of local spins and the DM interaction is given by the intrinsic spin current[2]. Using these two approaches, we calculate the DM interaction for $Mn_{1-x}Fe_xGe$, which is a typical skyrmion host material, and show how our methods explain the experiments.
This work was done in collaboration with R. Arita, N. Nagaosa, G. Tatara and T. Kikuchi.

[1] T. Koretsune, N. Nagaosa, and R. Arita, Sci. Rep. **5** 13302 (2015).

[2] T. Kikuchi, T. Koretsune, R. Arita, and G. Tatara, Phys. Rev. Lett. **116** 247201 (2016).

17a-4

Superconductivity of chromium thin film

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From the point of view not only of pure research but also of applied and practical one, there are many examples of superconducting thin films. But almost all of them were those in which superconductivity disappears when the film thickness is made thin [1]. It is likely to make a superconducting electron pair when it becomes thinner than the mean free path of electrons.

On the other hand, Schmidt et al. reported that thin films of chromium (Cr) metal suppress the antiferromagnetic ordering and become superconductive at $T_C \sim$ 1.5 K [2]. Taking account that the bulk Cr is an antiferromagnet below T_N = 311 K and does not show superconductivity [3], the relationship between film thickness and existence of superconductivity of Cr is opposite to the other examples of superconducting thin films.

Assuming that the magnetic correlation interaction is suppressed by controlling the film thickness, Cr may show a magnetic order-disorder transition tuned by the film thickness, and unconventional superconductivity may occur at the quantum critical point of $T \rightarrow 0$, where an electron pair appears due to quantum fluctuation. Generally, the three-dimensional electron system such as bulk compounds and two-dimensional one such as thin films are described by completely different Hamiltonian. That is, film thickness is an effective parameter that can directly control dimensionality, and it is interested in whether Cr is the first case of the new quantum phase transition tuned by film thickness [4]. In the present study, we perform precise electrical resistance measurements of chromium thin films to clarify the electronic state in a wide temperature range.

[1] H. M. Jaeger, D. B. Haviland, B. G. Orr, A. M. Goldman, Phys. Rev. B, **40** (1989) 182.
[2] P. H. Schmidt, R. N. Castellano, H. Barz, B. T. Matthias, Physics Letters, **41A** (1972) 367.
[3] M. Ohashi, G. Oomi, Jpn. J. Appl. Phys., **48** (2009) 070221.
[4] M. Ohashi, K. Ohashi, M. Sawabu, M. Miyagawa, T. Kubota, K. Takanashi, Physics Letters A, **380** (2016) 3133.

17p-1

Application of spin-polarized positron spectroscopy to some ferromagnetic systems

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Spin-polarized positron spectroscopy may be a unique tool for studying spin-polarized electronic states. That is, this method is applicable to the investigations of (i) spin-polarized electron momentum distribution (SP-EMD) of bulk system which connects with the band structure, (ii) magnetic moments associated with vacancy defects that cause so-called d^0 ferromagnetism of semiconductors, and (iii) surface spin-polarization of ferromagnets and also strong spin-orbit coupling systems. In this talk, I introduce recent results on SP-EMDs of Heusler alloys ($Co_2Mn(Fe)Si(Al)$, NiMnSb), spin-polarizations of vacancies in ZnO and GaN, and spin injection from Co to single layer graphene and BN.

Open circles in Fig. 1 shows the SP-EMDs measured for Co_2MnSi and Co_2MnAl polycrystals. The SP-EMD of Co_2MnSi is composed of a low momentum peak around p_z=0 m_0c and a high momentum shoulder around p_z=10x10^{-3} m_0c. Contrary, the intensity of the SP-EMD of Co_2MnAl is significantly lost around p_z=0 m_0c. The measured SP-EMDs are in good agreement with a package code (ABINIT) band structure calculation. This first suggests that the calculation was done with enough precision. The peak of the SP-EMD of Co_2MnSi at p_z=0 m_0c is explained as the existence of sp-like band dispersion of majority spin bands near the Fermi level. Whereas, the valley of the SP-EMD of Co_2MnAl at p_z=0 m_0c is explained as the absence of such bands.

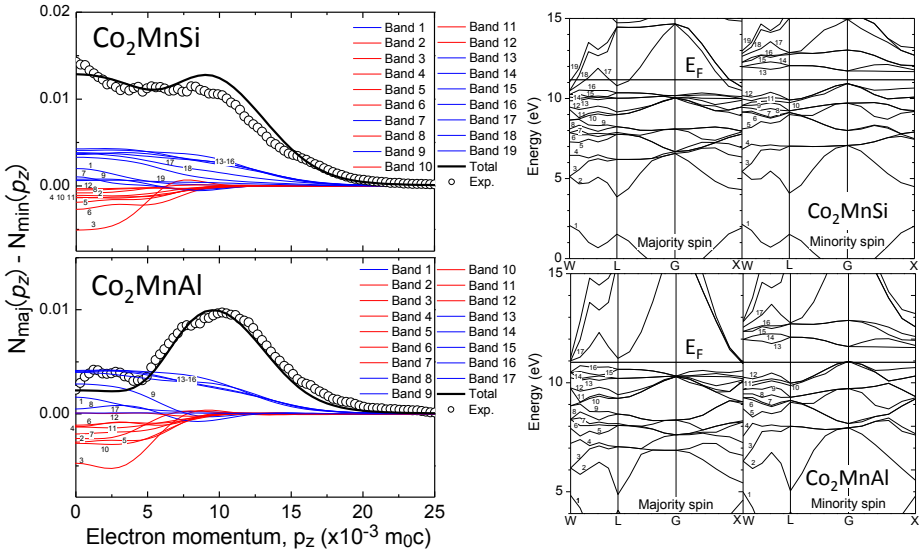

Figure 1 Spin-polarized electron momentum distributions obtained for Co_2MnSi and Co_2MnAl

17p-2

First-principles study on intrinsic and extrinsic anomalous Hall conductivity of transition metal alloys

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The anomalous Hall effect (AHE) is one of the unique phenomena in ferromagnetic metals and has been investigated from physical interests for a long time. Recently, this effect has attracted particular attention from the field of the "spin orbitronics" due to its close connection with the spin Hall effect, which is expected to be applied for a new mechanism of magnetic reversal with lower energy consumption. However, the systematic understanding of AHE in real metals still has not been accomplished.
One of the main complexities of AHE in real metals is its multi-mechanisms. The intrinsic mechanism connects with the Berry phase and has finite conductivity even in the no-scattering system. In contrast, the extrinsic mechanism is purely scattering effect and become divergent in the low impurity limit. Recently, reflecting these backgrounds, the first-principles procedure for evaluation of the anomalous Hall conductivity (σ_{xy}) including both the intrinsic and extrinsic mechanisms was presented based on the Kubo-Streda formula [1], which is within the linear-response theory, in the disordered systems [2,3,4].

In the present study, we performed first-principles calculation of σ_{xy} based on Kubo-Streda formula using Tight-binding Linear Muffin-tin Orbital (TB-LMTO) method. Figure 1 shows the calculated each part of σ_{xy} in FePt alloy as a function of degree of order (S) [5]. From this result, we confirmed that the skew-scattering part of σ_{xy} actually tends to diverge in the limit of low impurity limit (S $\fallingdotseq$ 1 in Fig. 1), whereas, the intrinsic and side-jump parts keep the steady values in the same limit.

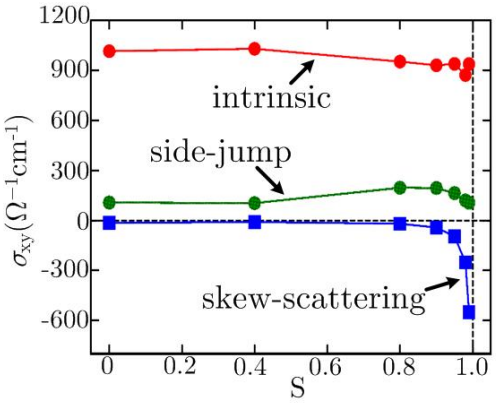

Figure 1: chemical order parameter(S) dependence of σ_{xy} in FePt alloy

[1] P. Streda, J. Phys. C: Solid State Phys., **15**, L717-L721 (1982)
[2] S. Lowitzer, D. Ködderitzsch, and H. Ebert, Phys. Rev. Lett., **105**, 266604 (2010).
[3] I. Turek, J. Kudrnovský, and V. Drchal, Phys. Rev. B, **86**, 014405 (2012)
[4] I. Turek, J. Kudrnovský, and V. Drchal, Phys. Rev. B, **89**, 064405 (2014)
[5] K. Hyodo, Y. Kota, and A. Sakuma, Phys. Rev. B, **94**, 104404 (2016)

17p-3

Computational Design of Transition Metal Magnets with Large Magnetocrystalline Anisotropy

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The magnetocrystalline anisotropy energy (MAE) is one of the technologically most important intrinsic magnetic properties. It is crucial in a wide range of applications, ranging from permanent magnets to magnetic storage devices. The MAE is often strong in rare-earth or actinide compounds, while obtaining a large MAE in 3d-based magnetic materials is challenging due to the weak spin-orbit interaction. On the other hand, 3d based compounds would often be preferred in applications. In this talk, potential routes towards increased MAE in transition metal magnets are discussed and explored using computational methods, largely based on density functional theory (DFT). Alloying and inducing tetragonality with C or B dopants is discussed as a path towards increased MAE in FeCo alloys [1,2,3]. The possibility to improve the MAE of 3d based compounds by including some 5d elements with stronger spin-orbit interaction is also considered. This is attempted by including small amounts of 5d impurities in 3d based compounds, such as $(Fe_{1-x}Co_x)_2B$, where a significant increase in the MAE and good agreement with experiment is found [4]. Uniaxial 3d-5d compounds, such as $Fe_2Ta_{1-x}W_x$ [5], are also discussed.

[1] E. K. Delczeg-Czirjak *et al.,* Physical Review B **89**, 144403 (2014).
[2] L. Reichel *et al.*, Journal of Applied Physics **116**, 213901 (2014).
[3] L. Reichel *et al.*, J. Phys.: Cond. Matt. **27**, 476002 (2015).
[4] A. Edström *et al.*, Phys. Rev. B **92**, 174413 (2015).
[5] A. Edström, arXiv:1612.06802.

17p-4

Voltage control of magnetization using magnetoelectric antiferromagnet Cr_2O_3 sputtered thin film

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Cr_2O_3 is the first material which the magnetoelectric (ME) effect is observed in 1960s [1]. However due to its small magnetoelectric coefficient α, i.e. small electric field induced magnetic moment $M = \alpha E$, the practical application was not immediately realized. After that, the ME effect in Cr_2O_3 has captured renewed attention because the electrical switching of perpendicular exchange bias (PEB) has been demonstrated in bulk Cr_2O_3 single crystal/ferromagnet exchange coupling systems in 2005 [2,3]. More recently, the PEB switching was demonstrated in Cr_2O_3/spacer/Co all thin film system deposited by the sputtering method [4-6]. Since then, the system has received considerable attentions toward application of an electric writing ultra-low energy consumption storage/memory applications. The electric switching of PEB can be achieved by following mechanism. By applying parallel (anti-parallel) electric (E) and magnetic field (H), the antiferromagnetic domain of Cr_2O_3 align as ↑↓↑↓ (↓↑↓↑). If we apply fixed positive H and changing the direction of E from positive to negative, we can switch the direction of surface spin of Cr_2O_3 from up (↑) to down (↓). In addition, the surface spin information can be transferred to neighbor ferromagnet via exchange coupling. Thus by combining both the ME effect and PEB, we can achieve electric control of magnetization. After the observations of the electric switching of PEB in Cr_2O_3 thin film system, we've tried to improve the material properties; reduce the switching electric field [7], enhance magnetic anisotropy [8], propose structure to enhance T_N of Cr_2O_3 [9] etc. Moreover recently Cr_2O_3 has received renewed interest as an antiferromagnet, reflecting the development of new detection/manipulation techniques. For example, ferromagnet free purely antiferromagnetic memory was proposed [10]. Spin Seebeck effect was also measured [11]. We will mainly present our results about the voltage control of magnetization in Cr_2O_3/Co exchange biased thin film system, with introducing other recent renewed interest.

This work was partly funded by JSPS KAKENHI Grant Number 16H05975 and ImPACT Program of Council for Science, Technology and Innovation (Cabinet Office, Japan Government).

References

[1] I. E. Dzyaloshinskii, *Sov. Phys. JETP* **10**, 628 (1960).
[2] P. Borisov et al., *PRL* **94**, 117203 (2005).
[3] X. He et al., *Nat. Mater.* **9**, 579 (2010).
[4] T. Ashida TN et al., *APL* **104**, 152409 (2014).
[5] T. Ashida TN et al., *APL* **106**, 132407 (2015).
[6] Y. Shiratsuchi et al., *Mater. Trans*. **57**, 781 (2016).
[7] M. Al-Mahdawi, TN et al., *arXiv* : 1608.02390.
[8] N. Shimomura TN et al., *arXiv* : 1605.03680.
[9] Y. Kota et al., *IEEE Trans. Magn*. **50**, 2505404 (2014).
[10] T. Kosub et al., *Nat. Commun.* **8**, 13985 (2017).
[11] S. Seki et al., *PRL* **115**, 266601 (2015).

Investigation of spin dependent van der Waals density functional approach

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First-principles calculation, which is based on density functional theory (DFT), is one of established method to analyze condensed materials. It also come to be used for material designs which leads to promote development of novel materials. Investigation of novel materials, *i.e.* they have an unclear physical property, by using fist-principles approach, is required the sufficient reliability computational method. However the computational accuracy in DFT calculation depends too much on the approximation of exchange and correlation energy. Indeed, the commonly and frequently used approach, based on such as local density approximation or generalized gradient approximation, cannot describe van der Waals (vdW) force properly.

The van der Waals density functional (vdW-DF) method, which is one of promising methods to overcome the problem, has been proposed by Dion et al [1]. We have proposed the extension of vdW-DF to spin-polarized (magnetic) systems, vdW-DF-SGC (SGC means spin-polarization-dependent gradient correction), and demonstrated the usefulness [2]. We also focused on the effect of SGC which described the spin dependent semi-local electron correlation effect, and found that it plays an important role in antiferromagnetic interactions.

Another spin van der Waals method (svdW-DF) was developed in 2016 [3]. The relation between vdW-DF-SGC and svdW-DF should be clarified in several applications. Therefore we also implemented this method in the house-DFT code, and investigated the oxygen systems and the absorption system which contains magnetic materials, namely, graphene on Ni(111) surface. Comparing these results with those of our method, we found that the svdW-DF also corrected the antiferromagnetic coupling and gave almost the same binding property as the vdW-DF-SGC.

[1] M. Dion et al., Phys. Rev. Lett. **92**, 246401 (2004).

[2] M. Obata et al., J. Phys. Soc. Jpn. **82**, 093701 (2013); **84**, 024715 (2015).

[3] T. Thonhauser et al., Phys. Rev. Lett. **115**, 136402 (2015).

Chiral magnetism in $CsCuCl_3$ probed by polarized neutron scattering and muon spin rotation

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Numerous experimental and theoretical studies have focused attention on chiral magnets with antisymmetric Dzyaloshinskii-Moriya interaction, because they provide opportunities to observe stable magnetic topological structure such as whirls of magnetization called skyrmions and a spiral helimagnetic order. Most of inorganic chiral magnetic materials form racemic-twinned crystals, having the right and left-handed crystalline domains in a specimen so that it is difficult to study the relation between crystallographic chirality and chirality of magnetic structures. Recently, our group succeeded in controlling the crystallographic chirality and obtained cm-sized single crystals of chiral helimagnet $CsCuCl_3$ with homo-chirality, namely, enantiopure crystals. In order to clarify the relation between crystallographic chirality and that of magnetic structures in $CsCuCl_3$, we performed polarized neutron diffraction and muon spin rotation measurements.

We found that the intensity of the magnetic satellite peak at (1/3, 1/3, 6-δ) and (1/3, 1/3, 6+δ) in both chiral crystals depends on the incident neutron spin polarization [1]. Moreover, the muon spin precession frequencies behaves the same temperature dependence in both crystals, suggesting that the right and left-handed samples are a pair of complete isomers in terms of both crystallographic and magnetic structures [2]. These investigations revealed that there is a one to one relationship between the structural and magnetic handedness in $CsCuCl_3$; namely the right-handed crystal structure has a right-handed spiral magnetic structure, and left-handed crystal has a left-handed spiral magnetic structure. In the presentation, we shall discuss in detail the results of the two experiments.

[1] Y. Kousaka *et al*., J. Phys.: Conference Series **502**, 012019 (2014).
[2] K. Ohishi *et al*., JPS Conf. Proc. **8**, 034006 (2015).

18a-2

Quantum simulation for the motion of positive-muon in materials and its application for Mu-SR spin state analysis

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Abstract

Mu-SR is one of the powerful tools to observe the spin states of atoms in materials [1]. It is important to know the positive-muon sites, which are the stable or metastable positions of positive-muon in the materials, because the spins of muon at such sites can detect the magnetic field or effective magnetic interaction with the electron spin in the materials. However, it is difficult to get information about positive-muon sites using experimental methods. In this case, computer simulations may give such information, which can complement the Mu-SR data.

Positive muon has the same charge and spin with proton, and has mass 1/9 that of a proton. In materials, positive muon behaves as the nucleus of the very light hydrogen isotope. Density functional theory based first principles calculation is one of the most successful and powerful methods that can be used to decide the atomic positions in materials. For the case of atom with small mass such as hydrogen, its nuclei should also be treated in a quantum-mechanical manner, in addition to electrons. The quantum behaviors of the small mass nuclei have crucial roles in the properties of materials. We have been developing a quantum simulation code "NANIWA" for small mass atom nuclei on solid surfaces, in subsurfaces, and in bulk crystals [2-6], which can also provide the positive-muon sites in material.

In the workshop, we will introduce our simulation method and show its results in comparison with their corresponding experimental data. And we will also discuss its possible application for Mu-SR spin state analysis.

References

[1] S.F.J.Cox, Rep. Prog. Phys. 72 (2009) 116501.
[2] H. Kasai, et al., Progress in Surface Science, 44 (1993) 101.
[3] K. Nobuhara, et al., Surface Science, Vol. 507-510 (2002) 82.
[4] H. Nakanishi, Eds H. Kasai and M. C. S. Escaño (2016) *Physics of Surface, Interface and Cluster Catalysis.*, Bristol, UK, IOP Publishing, Ch.6-1.
[5] H. Kasai, H. Nakanishi, US Patent 8,140,467 B2 (2012), and JP Patent, 4774523 (2011)
[6] H. Kasai, H. Nakanishi, JP Patent, 5902495 (2016)

18a-3

Linear-scaling DFT study on the structural optimization and electronic properties of real size Ge/Si core-shell nanowires

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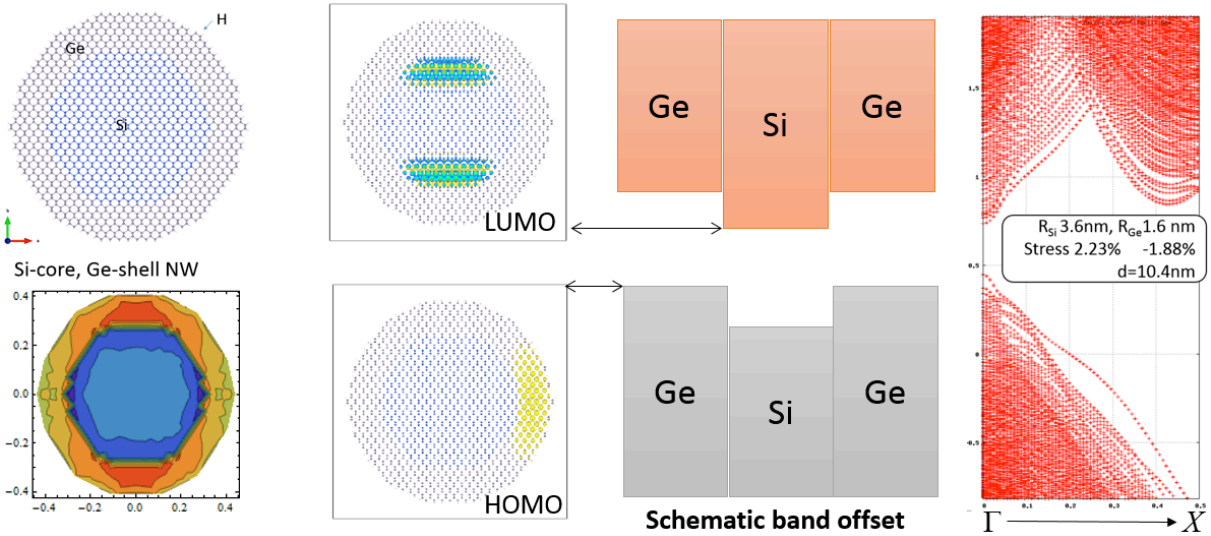
Silicon (Si) and germanium (Ge) core-shell nanowires (NWs) as one-dimensional nanomaterial have many attractive properties for next generation devices. Since there is a lattice mismatch between Si and Ge, we expect the structure of the NW strongly depends on the diameter of the core and/or the thickness of the shell. Therefore, we also expect that the electronic properties can be controlled by varying the diameter of the core and/or the thickness of the shell in the core-shell NWs. It is very important to clarify and understand how the strains are distributed in the actual NWs.

In this work, using our linear-scaling or O(N) DFT code CONQUEST, we performed structure relaxation of the core-shell NWs whose diameters are up to 15nm. The code can perform DFT calculations on million-atom systems and we can calculate the structural and electronic properties of the NWs with the actual size. In this talk, I will report the reliability of large scale DFT calculations in current system, the strain distributions, and the band structures. The dependence between strain distribution and the Kohn-Sham eigen orbitals will be also discussed.

This work is done in collaboration with the experimental group headed by Dr. N. Fukata at NIMS-MANA, and Dr. S. Arapan, Dr. Y. Futamura, Prof. T. Sakurai (Tsukuba Univ.), Dr. C. O'Roulke and Mr. S. Mujahed (UCL) for theoretical calculations.



18a-4

Nonreciprocal propagation of elementary excitations in noncentrosymmetric magnets

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Simultaneous breaking of spatial inversion and time-reversal symmetries completely lifts the degeneracy between $+k$ and $-k$ states of elementary excitations in solids. In this case, the decay rate and phase velocity depends on the sign of k, and, hence, the propagation of the elementary excitation becomes nonreciprocal. The photonic nonreciprocity, which is denoted as magnetochiral or optical magentoelectric effect, has been investigated extensively in the last two decades. Here, we experimentally study the nonreciprocal propagation of magnons and acoustic waves as well as microwaves in noncentrosymmetric magnets [1-5].

[1] Y. Okamura, Y. Onose *et al.*, Nature communications 4, 2391 (2013).
[2] Y. Nii, R. Sasaki, Y. Iguchi, Y. Onose, arXiv. 1605.07414 (J. Phys. Soc. Jpn. Editor's choise, *in press*).
[3] Y. Iguchi, Y. Nii, Y. Onose, arXiv:1607.06889.
[4] Y. Iguchi, S. Uemura, K. Ueno, Y. Onose, Phys. Rev. B 92, 184419 (2015).
[5]R. Sasaki, Y. Nii, Y. Iguchi, Y. Onose, Phys. Rev. B 95, 020407(R) (2017).

Theory of spin current generation

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Spintronics is a field aimed at controlling and using the spin degree of freedom of the electrons. In this field, the spin current, which is the flow of the spin angular momentum has been extensively studied. Particularly, it is expected that a device with suppressed energy loss due to the Joule heating can be realized by using the spin current.

In order to develop a device using the spin current, it is necessary to establish the method of spin current generation and to improve its efficiency. The spin pumping and the spin Seebeck effect, i.e., generation of the spin current in the bilayer system of a ferromagnet and a metal by applying an oscillating magnetic field and a temperature gradient, respectively, have attracted much attention. Since there is no charge transfer at the interface, the spin pumping and the spin Seebeck effect are free from the impedance mismatch problem which often reduces the spin injection into semiconductors. The generated spin current is converted into an electric signal by the spin-orbit interaction in the metal. This phenomenon of conversion from the spin current into the charge current is referred to as the inverse spin Hall effect.

In this talk, we show that theoretical investigation of the spin pumping and the spin Seebeck effect and that material dependence of the spin current [1-3]. In addition, we show the theoretical study of the inverse spin Hall effect in half-metallic ferromagnets [4] where the conduction electrons are completely spin-polarized. Based on our results, we propose the several mechanisms for efficient spin current generation.

References

[1] Y. Ohnuma *et al*., Phys. Rev. B **89**, 174417 (2014).
[2] Y. Ohnuma *et al*., Phys. Rev. B **87**, 014423 (2013).
[3] S. Geprägs *et al*., Nat. Commun. **7**, 10452 (2016).
[4] Y. Ohnuma *et al*., Phys. Rev. B **94**, 184405 (2016).

Numerical simulation for dynamical elastic contact problem

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The purpose of this work is to present a model which describes dynamical elastic contact. We aim for the model which can reproduce a collision of rolling ball, a motion of tire on road, and stick-slip with PDEs. Stick-slip occurs, for example, from an inter action of roller and paper (sheet feeder). It is easy to suppose that friction and restitution coefficient are related with this phenomenon, but it seems that another are related with. We adopt new points which are adhesion force, surface tension force, and hysteresis of friction. We investigate how to describe these points as PDEs. In this presentation, especially, we focus on surface tension force.

In order to obtain numerical solutions, we employ discrete morse flow(DMF) which is better for global constrain. Let $\Omega \subset \mathbb{R}^2$ be an open domain with smooth boundary and $\Gamma_D \cup \Gamma_K = \partial\Omega, \Gamma_D \cap \Gamma_K = \emptyset$. $(u = (u^1, u^2), x = (x^1, x^2))$. σ and ε are stress tensor and strain tensor respectively.

$$J_m(u) = \int_\Omega \frac{|u - 2u_{m-1} + u_{m-2}|^2}{2h^2}\, dx + \frac{1}{2}\int_\Omega \sigma(u) : \varepsilon(u)\, dx + S(u), \qquad m = 1, 2, \cdots$$

$$\mathcal{K}_m := \{z \in H^1(\Omega; R^2); z = g_m \text{ on } \Gamma_D, z^2(x) + x^2 \geq 0 \text{ for } x \in \Gamma_K\}$$

u_{-1} and u_0 are given functions, $u_m,\ m = 1, 2, \cdots$ is a minimizer of J_m on $\mathcal{K}_m$. surface tension force is defined by

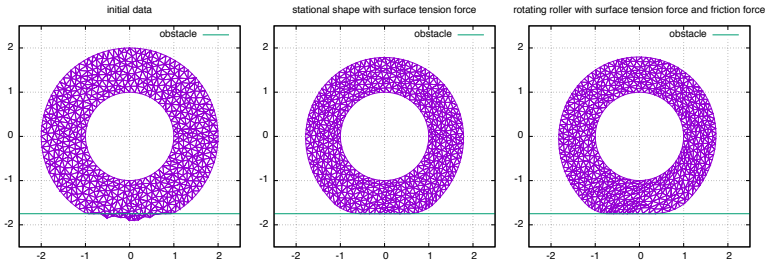
$$S(u) := \int_{\Gamma_K} \gamma_1 |p_s|\, ds + \int_{\Gamma_K} \gamma_2 \chi_{\{p^2>0\}} |p_s|\, ds$$

where $p(x) = u(x) + x$ for $x \in \overline{\Omega}$. $\gamma_1 = \gamma_{SL} - \gamma_{SG}$ and $\gamma_2 = \gamma_{LG} - \gamma_{SL} + \gamma_{SG}$ are surface tension coefficients. The minimizer satisfies the followings:

$$\begin{cases} \sigma(u)n = -\gamma_{LG}\kappa|p_s|\nu & \text{on } \partial\Omega \cap \{p^2 > 0\} \\ (\sigma(u)n)^1 = 0, \quad (\sigma(u)n)^2 \geq 0 & \text{on } \partial\Omega \cap \{p^2 = 0\} \\ \gamma_{LG}t^1 = \gamma_{SL} - \gamma_{SG} & \text{on } \partial\Omega \cap \partial\{p^2 > 0\} \end{cases}$$

where n is an unit outer normal vector of $\partial\Omega$, $t := p_s/|p_s|$, and $\nu = -t_s/|t_s|$.

Numerical result of a weak coupling with Coulomb friction model



For numerical results, we could not observe a vibration which likes stick-slip. In future, we focus on adhesion and hysteresis of friction.

SMOOTHED PARTICLE HYDRODYNAMIC SIMULATION OF ACCRETION DISK IN CATACLYSMIC VARIABLE

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ABSTRACT

An investigation on accretion disk in cataclysmic variable stars (CVs) becomes an interesting phenomenon in astrophysics since one of its effects, the oscillation of the brightness of the light curve from photometric has been observed. Since the disk of CVs is the brightest component of the system, it is believed that the oscillation might come from mass transfer of the accretion process. In this research, we use an SPH (Smoothed Particle Hydrodynamics) method to visualize the generation process of an accretion disk in Cataclysmic Variables.

Since introduced by Lucy (1977) and Gingold & Monaghan (1977), SPH is widely used to simulate many astrophysical phenomena. SPH is a Lagrangian method which discretizes the continuum into a set of particles. In this research we simulate the system of binary stars with mass ratio 1:0.08 $M_{\odot}$ and short rotation period (1000s). For the sake of simplicity, we consider our continuum as an ideal gas, and ignoring the magnetic effect of the stars. Variation of bolometric luminosities is determined by summation of the changes in the internal energies of all particles in each time steps.

Keywords: accretion, accretion disks - hydrodynamics - binaries: close - methods: numerical - novae, cataclysmic variables

First-Principles Study of Electronic, Magnetic, and Optical Properties of Nickel Cobaltite: DFT and QSGW methods

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Nickel cobaltite ($NiCo_2O_4$) is one candidate of novel materials that could be engineered in many ways to exhibit different properties. For example, by utilizing temperature growth of less than 450^{o}C, ones can acquire metallic-ferrimagnetic $NiCo_2O_4$ thin film. On the contrary, with more than 450^{o}C, we would acquire that film as non-magnetic insulator [1]. This uniqueness is believed to come from the competition between double exchange interaction among cations with different charges and superexchange interaction among those with same charges [2]. Nickel cobaltite is also predicted to be half metallic, due to the existence of a band gap on its majority-spin state band.

We employed first-principles density functional theory (DFT) and quasiparticle self-consistent GW method (QSGW) to elucidate electronic, magnetic and optical properties of different types of $NiCo_2O_4$ predicted bulk structures. There are some discrepancies arising between GGA and QSGW methods in addressing double exchange and superexchange interaction. In this regards, QSGW described more accurate electronic structure. These results also compared with those of more well-known materials, i.e. Fe_3O_4 and Co_3O_4.We considered three possible bulk structures of Nickel cobaltite, namely normal spinel, type-A inverse spinel, and type-B inverse spinel. Both GGA and QSGW predicted half-metallicity of type IB with indirect band gap at majority channel exhibited by Table 1. In addition, optical properties of $NiCo_2O_4$ also investigated by calculating dielectric function and comparing it with experiment optical absorption spectra.

Table 1. Band gap in the majority-spin state for different $NiCo_2O_4$ structure probabilities (with experiment data).

Method	**Band gap of different Spinel Structures (eV)**		
	Normal	Type-A inverse	Type-B inverse
GGA	0.89	0.87	0.90
QSGW	1.07	1.25	1.36
Expt.[3]	0.38 – 1.42 (Indirect)		

[1] P. Silwal, et al., Applied Physics Letters, **100**, (2012), 032102.

[2] Y. Bitla, et al., Scientific Reports, **5**, (2015), 15201.

[3] K. Dileep, et. al., J.Phys. D: Appl. Phys. **47**, (2014), 405001.

Holonomic Gradient Method for the Distribution Function of the Largest Root of Complex Non-Central Wishart Matrices

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We evaluated the outage probability of multiple-input-multiple-output (MIMO) systems employing maximal ratio combining (known also as beamforming systems) and operating over Rician-fading channels using a relatively new numerical method called Holonomic Gradient Method (HGM).

In conventional wireless communications, a single antenna is used at the source and another single antenna is used at the destination. In some cases, this gives rise to problems with multipath effects which can cause a reduction in data speed and an increase in the number of transmission errors. One of the solutions to this problem which is very popular among telecommunication engineers is the use of two or more antennas, hence the MIMO system.

The outage probability is an important statistical measure to assess the quality of service provided by the system. It is defined as the probability of failing to achieve a specified Signal to Noise Ratio (SNR) value sufficient for satisfactory reception. It is known that the outage probability can be expressed as the Cumulative Distribution Function (CDF) of the largest eigenvalue of a non-central Wishart Matrix.

In the past years, there have been several attempts to compute the outage probability using method such as Monte-Carlo or power series expansion [1]. However, those computations are relatively slow. This disadvantage becomes more apparent especially when we want to perform a computation over several threshold values or when a large number of antennas is involved.

We would like to develop a new method that can perform this computation for several value of quickly for a large number of antennas. We found that outage probability of MIMO system can be expressed as a holonomic function. Thus, we use this fact and use HGM as this method is known to be faster and more efficient than other alternatives in doing a computation involving a holonomic function [2].

The HGM consists of three steps: (1) Finding a holonomic system satisfied by the function and translating it to a Pfaffian system. (2) Finding an initial value vector for the Pfaffian system. (3) Using the obtained Pfaffian system to evaluate the function numerically at several points by the Runge-Kutta method.

Our result shows that HGM is a faster and more efficient method than Monte-Carlo and power series expansion for computing the CDF of the largest eigenvalue of a non-central Wishart Matrix. It is shown by the computation time and the number of antennas that this method can handle without compromising the computation time too much. As a validity check, we compare our result with the one that appears in some previous research publication. We found that the graph of our result agrees with the one in the paper.

References

[1] Ming Kang, Mohamed-Slim Alouini, Largest Eigenvalue of Complex Wishart Matrices and Performance Analysis of MIMO MRC Systems, IEEE Journal on Selected Areas in Communications, **21** (2003), No. 3, 418–426.

[2] Hiroki Hashiguchi, Yasuhide Numata, Nobuki Takayama, Akimichi Takemura, Holonomic gradient method for the distribution function of the largest root of a Wishart matrix, Journal of Multivariate Analysis, **117**, (2013) 296–312

First-principles study on θ-phase in solid oxygen

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Oxygen molecules, which are indispensable to living organisms, provide interesting themes not only in the field of earth science, biology, chemistry, but also in condensed matter physics. This is because oxygen molecule has rare features with spin quantum number S=1 among simple homonuclear diatomic molecules, and also because both of van der Waals force and magnetic intermolecular force play an important role in the condensation of molecules. As a consequence, the crystal structure is determined under a subtle balance. Solid oxygen changes its crystal structure by the external parameters such as temperature and pressure. Seven phases ($\alpha, \beta, \gamma, \delta, \varepsilon, \zeta, \eta$) have been discovered so far.

Recently, experimental studies on the one-turn coil method indicated that the magnetization rapidly changes under a high external magnetic field (around 120 T) [1]. It is suggested that this has undergone a phase transition to a new structure (θ-phase). This phase, in which there are ferromagnetic correlation and intermolecular sequence like S-type or X-type, is expected to be a different phase from conventional solid oxygen. In order to elucidate its structure, we investigated several types of crystal structures by using the first-principles approach which employs the vdW density functional as the exchange correlation energy.

We calculated the cohesive energy of dry ice structure and iodine structure considered as candidates for θ-phase, assuming ferromagnetic state. The volume of θ-phase, which expands under a strong magnetic field, was estimated to be about 15% larger than that of α-phase. This result corresponds well to those of experimental data, indicating that the computational approach supports the dry ice structure as the most probable candidate.

[1] T. Nomura et al., Phys. Rev. Lett., **112**, 247201 (2014).

Title : Numerical study of an adaptive Lagrange-Galerkin scheme for pure convection problems

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Abstract :
The Lagrange-Galerkin (LG) scheme is a combination of the finite element method and the method of characteristics, and is known as one of the powerful numerical methods for flow problems.
Introducing an adaptive mesh refinement technique, we have implemented an adaptive LG scheme for pure convection problems.
In the poster numerical results of the scheme are presented and they are studied from the view points of computation cost and accuracy.

Theoretical study on multi-functional Fe/MgO interface: investigation of perpendicular magnetic anisotropy origin

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Multi-functional thin film of iron/MgO interface has a lot of interesting physical properties and potential application for magnetic and magnonic devices. Its unique magnetic characteristic, perpendicular magnetic anisotropy, voltage/spin-current controlled magnetic anisotropy, also unique spin structure with voltage controlled Dzyaloshinskii-Moriya interaction [1]. This feature is promising for information technology device, especially for high density and low power consumption data storage. Another possible application of the spin waves in this interface can be used for higher frequency (more than Tera Hertz) of RF devices [2], because its have several orde of magnitude shorter wavelength. The latter thin film also can be used for information bus and logic gate for future integrated signal-processing magnetic device.[1]

Such data sotrage/memory can be created by utilizing novel concept of the voltage controlled perpendicular MTJ. Even though the technology is seems to be mature, but there is still a lot of room for improvement. For example, the large perpendicular magnetic anisotropy (PMA) is required to keep the device stable under thermal fluctuation and high temperature of fabrication process. Current value of PMA is below 1 mJ/m^2 [3], this still need to be improved in order to ensure the stability and prevent deterioration of the memory cell due to aging and disturbance of external field.

This work performed basic re-investigation of this interface to find the mechanism of how PMA can be found. The calcualtions of density functional theory (DFT) and dipole interaction energy correction were carried out to estimate the magnetic anisotropy energy (MAE) of ultrathin multilayer iron film, Fe/MgO interface, and the Fe/MgO interface with Chromium (Cr) buffer layer. The high density of $\mathbf{k}$ sampling point with spin-orbit interaction was taken into account in the DFT.

Calcualtion reslut showed the interface system demonstrates high perpenducular magnetic anisotropy energy. The electronic structure near the Fermi level provides important information to the magnetic anisotropy properties. Basic mechanism of perpendicular magnetic anisotropy based on second order perturbation theory is used to explain the large positive contribution to MAE. Our results encourage experimentalist to challenge more advanced fabrication to realize various properties on MAE.

This work was supported by ImPACT Program of Council for Science, Technology and Innovation (Cabinet Office, Japan Government) and by the Kanazawa University SAKIGAKE Project.

[1] K. Nawaoka et al., Appl. Phys. Exp. **8**, 063004 (2015).
[2] V. V. Kruglyak et al., J. Phys. D: Appl. Phys. **43**, 264001 (2010).
[3] T. Nozaki et al. (2016). Phys. Rev. Appl. **5**, 044006 (2016).

First principles calculation of magnetic anisotropy energy on double interfaces slab systems of X/Fe/MgO

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There is an important purpose to develop a non-volatile random access memory due to advanced information oriented society. Magnetic random access memory (MRAM) is one of the most desirable candidates. MRAM drives based on spin orientation of memory cells and the energy barrier to spin orientation is called magnetic anisotropy energy (MAE). High MAE is necessary for thermal resistivity to keep the memory [1], but it consumes high energy for data rewriting. Magnetoelectric random access memory (MeRAM) can variate MAE by electric field and the rate of variation is called voltage control magnetic anisotropy (VCMA) [2]. High VCMA is desirable to achieve replacing current RAM. The MAE is originated from spin-orbit coupling (SOC) and magnetic dipole-dipole interaction (MDI). Recent magnetic memory requires a perpendicular magnetization due to realizing a small size of memory cell. In this work, we focus on the contribution of SOC because the MDI contributes to the favor of in-plane magnetization and is not expected to change under the electric field. The Fe/MgO interface is essential for MeRAM owing to several reasons, e.g. high tunneling magnetic resistance ratio, easy to fabricate, perpendicular magnetization, etc. However, it is difficult to analyze the internal electronic structure experimentally. So far, many theoretical approaches have been accomplished in the properties of MAE and VCMA [3,4].

We studied the slab systems of X/Fe/MgO (metal for X) with double interfaces. Such system keeps the Fe/MgO interface and has possibility to improve MAE by intrinsic deflection of the under layer (X). We estimated MAEs and VCMAs in X/Fe/MgO by using first-principles calculation and analyzed the electronic structures. The calculation results revealed a more concrete relation between electronic structures and MAE.

This work was supported by ImPACT Program of Council for Science, Technology and Innovation (Cabinet Office, Japan Government) and by the Kanazawa University SAKIGAKE Project.

[1] H. Ohno et al., Nat. Mater. **9**, 952 (2010).

[2] T. Nozaki *et al.*, Phys. Rev. Appl., **5**, 044006 (2016).

[3] M. Tsujikawa and T. Oda, Phys. Rev. Lett., **102**, 247203 (2009).

[4] D. Yoshikawa *et al*., Appl. Phys. Express, **7**, 113005 (2014).

Numerical simulation of contact problem of an elastic body with friction.

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We simulate contact problem of an elastic body with friction.

We introduce a way how to manage friction force artificially for the contact problem on the numeric.

Step 1: We find numerical solution of contact problem without friction.

Step 2: We consider an effect of friction from the solution of step 1.

Step 3: We set a boundary condition from the effect which we got in step 2.

Step 4: We find numerical solution of contact problem with the boundary condition of step 3.

We do numerical calculation in that way, and get the result considered that there is an effect of friction. However, we introduce friction on the numeric artificially, so the solution doesn't always satisfy the governing equation. We suppose that further studies are needed about how to deal with friction.

Hyperfine structure of muonium in GaN

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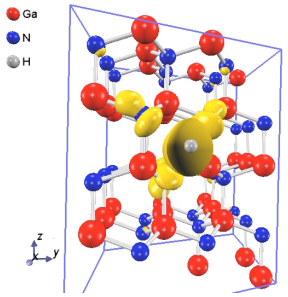
GaN is one of the important wide gap semiconductors. Its wide-band gap of 3.4eV affords its special properties for applications in electronic and optoelectronic devices, e.g., bright, highly efficient blue and green light-emitting diodes. It is well known that hydrogen contributes to passivation in the case of p-type doping. However, the electronic and atomic structures of mono-hydrogen in GaN is still unclear. An μSR experiment detected neutral paramagnetic muonium which has a shallow donor level, suggesting that hydrogen can be a shallow donor [1]. However, first-principles calculations indicate that hydrogen has a negative-U property [2,3].

An μSR experiment shows a strong anisotropic hyperfine structure[1], which is a key point to identify the atomic site of muonium which is expected to be the same as the stable site of hydrogen. In this study, we perform first-principles calculations of atomic and electronic properties of mono-hydrogen in GaN. We use generalized gradient approximation based on the density functional theory. A plane wave and pseudopotential are used. After that, we calculate hyperfine parameter by using all-electron calculation. Calculation code HiLAPW is used.

We find that the spin density is not simply localized at the hydrogen site, i.e., we find substantial spin densities at six N atoms which are near the hydrogen (see the figure). Furthermore, our calculation result reproduced anisotropic hyperfine parameter. Finally, this spin density distribution is expected to be consistent with the anisotropic hyperfine structure which was observed by using μSR.



[1] K. Shimomura, R. Kadono,, K. Ohishi, M. Mizuta, M. Saito, K. H. Chow, B. Hitti, and R. L.Lichti,. Phys. Rev. Lett. **100**, 111111 (2014).

[2] J. Neugebauer, and C. G. Van de Walle, Phys. Rev. Lett. **75**, 4452 (1995).

[3] A. F.Wright, Phys. Rev. B., **60**, R5101 (1999).

On the prediction of storm surge along the coast of Bangladesh

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Abstract

In this study, a shallow water model in Cartesian coordinates is developed to predict water level due to surge associated with a storm along the coast of Bangladesh. The developed equations are solved by a conditionally stable explicit finite difference method using an Arakawa C-grid. The coastal and island boundaries are approximated through proper stair step representations. Nested numerical technique is exercised to solve computational complexities as well as to save computational cost. A stable tidal regime is generated by forcing the sea level to be oscillatory with the most dominating constituent M_2 of the region of interest along the southern open boundary of the outer model. Numerical experiments are done with the two typical tropical storms April 1991 and AILA, 2009. The model results, so far obtained, are found to be in good agreement with the data by Bangladesh Inland Water Transport Authority (BIWTA) and some reported data.

3D simulation of crack propagation in an elastic body by a phase field model

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In this study, we perform 3D simulation of crack propagation in an elastic body by using FreeFem++. A phase field function is introduced in order to deal with crack growth flexibly.

In the simulation the dependency of the crack growth on the fracture toughness of the material is investigated.

An Implicit Boundary Integral Method for Laplace Problem

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Abstract

In this work, we consider boundary integral method to solve Laplace Dirichlet boundary problem. A few results from layer potential theory are used to construct a solution in the form of Double-Layer potential and Single-Layer potential for simple connected domain and for multi-connected domain. In order to find the density function and to construct the solution using boundary integral form, we use the idea of using Coarea formula and signed distance function representation to reformulate the boundary integral into a Riemann integral, such that it does not depend on any parameterization to describe the boundary. We also present the algorithm how to technically work with this method and show a few numerical results.

Keywords: Boundary Integral Method, Laplace Dirichlet problem, layer potential integral, level set method

FINITE ELEMENTS METHOD OF ERGODIC DISTRIBUTION FUNCTION FOR JAFFE MODEL

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ABSTRACT

Finite element method (FEM) has been widely used for solving in mathematical physics problem. In this study, we aim to use FEM to construct distribution function (DF) of stellar system. This method has been propose by Jalali (2007).The method is the generalization of Schwarschild's method. Unlike Schwarschild's method, this method provided a continuous DF and used two finite elements meshes, which is in configuration space and in action space. We also show the performance of FEM for spherically symmetric system by ergodic DF Jaffe model (Jaffe 1983). For the sake of simplicity, we generated the finite element mesh with simple double-node elements and linear interpolating functions.

Keywords : Finite element method, galaxies : structure, Jaffe model

NUMERICAL METHOD OF NONLINEAR BLACK SCHOLES EQUATION FOR AMERICAN OPTIONS PRICING

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ABSTRACT

The aim of this work is to calculate American options price with transaction costs from the Black Scholes model. Due to transaction costs, large investor preferences and incomplete markets, the classical Black Scholes model become unrealistic and results nonlinear, possibly degenerate, parabolic convection diffusion equations, where the volatility σ and the drift μ can depend on the time t, the stock price S or the derivatives of the options price (Ankudinova, 2008). In this work, several of volatility model will be used and compared to show the influence of transaction costs. The option pricing problem from nonlinear Black Scholes equation will be solved numerically using finite difference scheme combined with an operator splitting technique proposed by Ševčovič (2008).

Keywords : American options, Nonlinear Black Scholes equation, Volatility model

Computation of an inverse free boundary problem for a shape optimization method

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Numerical results of an inverse free boundary problem by a shape optimization method are presented and the efficiency is studied.

Many shape optimization methods have been proposed and studied. The traction method is known as one of the powerful methods for shape optimization problems. We apply the shape optimization method by traction method to an inverse free boundary problem.

A gradient flow structure of the Maxwell-type viscoelastic model and its finite element analysis

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The viscoelastic material has both viscosity and elastic effects.The Maxwell-type viscoelastic model is a system of partial differential equation defined by the series connection of spring and dashpot. This model can represent the stress relaxation phenomenon. In the poster we show the gradient flow structure of the model and propose a finite element scheme presenting the structure.

4 way-hexagonal symmetric crystalline method and 2 dimensional snow crystal model allowing collision / splitting

Yamaoka Ryohei,Tanaka Tomoe

In this research, we aim to construct a mathematical framework of 2 dimensional crystal growth model which allows side collision and split like snow crystal growth. Based on the mathematical formulation of the Crystalline method expanded to include splitting and collision of sides of hexagonal crystals made in the previous study, a quadrilateral growth model is considered. The numerical calculation is performed on the crystal growth model.

Development of a finite element method for a delamination model and its simulation

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In this study, we develop a finite element method for the delamination model proposed in [R.Scala , ESAIM : COCV , 2017] and present numerical results by the method. Two elastic bodies are glued by an adhesive and the delamination process induced by vibration in considered. The glue plays a role of "spring", and the delamination occurs when the difference of the displacements of two bodies exceeds a threshold.

Minimum energy state and gradient flow for interaction energy of particles

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Abstract

We are interested in minimum energy state of interacting particles. We have showed that there exist a minimum energy when the particles get a equilibrium state in one and two dimension, now we take a domain that contains particles and we want to find the minimum energy state by making the gradient flow from the function of energy of particles.