4．利用者論文一覧表

注：（1）この一覧は，平成 18 年 1 月から 18 年 12 月までの間に提出された利用者の論文別刷のうち，学協会誌，論文集等に掲載されたものを収録した。口頭発表による論文集別刷及び原稿プリント等（21 篇）は省いてある。
（2）共筆者がある場合は，当該別刷を提出した利用者に＊印を付した。
（3）掲載順序は，おおむね利用者の登録番号順による。

（1） *Kazuhiko OHMORI，Machie SAITOU，Guido EILERS and Masaaki MATSUI：**Magnetic Properties of Dilute Magnetic Semiconductor（CuIn）1-xMn2xS2**，Journal of the Physical Society of Japan，Vol.75，No.3，pp.034711-1 ～ 5（2006）

ABSTRACT：We have prepared samples of the dilute magnetic semiconductor $(CuIn)_{1-X}Mn_{2X}S_2$（x=0.0 ～ 0.3）and performed magnetic measurement. The magnetization curves were analyzed by considering two terms: the one was the contribution of the interactive Mn ions and the other one was the contribution of the isolated Mn ions. The decrease in the second contribution with the increase in Mn concentration was attributed to the decrease in the number of the isolated Mn ions and the increase in the number of Mn ion clusters such as pairs, triangles and networks. The dependences of the inverse magnetic susceptibilities on the temperature were measured and investigated using the above two terms. The observed data were ferrimagnetic like and the introduced formula for the dependences of the data on the temperature also showed the same tendency.

（2） *Takeo SOGA，Hiromitu NATUME，Takeshi MIYASAKA，Takashi HATTORI：**APPLICATION OF THE MOMENT EQUATIONS TO THE RAREFIED SUPERSONIC FLOW**，Computational Fluid Dynamics JOURNAL，Vol.13，No.30，pp.224 ～ 228（2004）

ABSTRACT：Moment equations derived from the Boltzmann equation were applied to the leading edge problem in the supersonic flow. Boundary conditions for the flow properties and higher order moments were derived by applying a generalized Grad's slip conditions. The moment equations were solved using Mac'Cormack's central difference scheme. Two-dimensional flow field on the flat plate was obtained in the scale of one mean free path. Numerical simulation with the mesh size of sub-mean free path yielded undesirable

numerical oscillation and in the vicinity of the leading edge at plate. On the other hand, numerical simulation with the mesh size of several mean free paths suggested that the moment equations were applicable to the hypersonic flow. The results with the mesh size of one mean free path showed a good agreement with the results of DSMC method. We then assured that moment equations with generalized slip boundary conditions were valid for the analysis of rarefied supersonic flows. It was expected that introduction of certain new types of artificial viscosity like the TVD scheme for further extend the applicable range of the moment equations.

（3） AKIRA YONEDA：**THE xyzr ALGORITHM SPECIALIZED FOR EIGENVIBRATION PROBLEM OF BORED AND LAMINATED OBJECTS**, Journal of Sound and Vibration, Vol.236, No.3, pp.431 ～ 441（2000）

ABSTRACT：We can determine elastic properties of an object from its eigenvibration frequencies, as long as a numerical calculation algorithm is available for the eigenvibration frequencies. The xyz algorithm developed by Visscher et. al.（1991）is an extremely versatile method applicable even for anisotropic, inhomogeneous, and irregular shaped objects except for bored and laminated systems. I examined the characteristics and performance of the original xyz algorithm, and succeeded in developing the new xyzr algorithm for bored and laminated sphere and cylinder. The accuracy and convergency of the xyzr algorithm are examined by comparing with the analytical solutions. Its high accuracy enables us to develop a new experimental technique obtaining elastic properties of liquids and soft materials accommodated in a solid tube; those elastic properties are deduced from the eigenfrequencies of the composite system.

（4） *T.Ikkai, T.Arii, K.Shimada：**Excimer Fluorescence as a Tool for Monitoring Protein Domain Dynamics Applied to Actin Conformation Changes Based on Circulary Polarized Fluorescence Spectroscopy**, Journal Fluorescence, Vol.16, pp.367 ～ 374（2006）

ABSTRACT：Fluorescence-detected circular dichroism（FDCD）was introduced into the study of protein conformation changes. Actin was used as a model protein which undergoes dynamic conformation changes as it polymerizes. Actin labeled with *N*-（1-pyrene）iodoacetamide（PIA）showed monomer fluorescence peak at 386 and 410 nm, and excimer fluorescence peak at around 480 nm. Excimer was formed by PIA-dimers labeled to different sites of amino acid residues. New information concerned with actin structural changes were monitored by fluorescence emission spectra excited with left- and right-circulary polarized light at 355 nm. FDCD intensities were shown as the

difference in the fluorescence emission ΔF, where $\Delta F=(F_L-F_R)/(F_L+F_R)$ denoting F_L and F_R as emissions obtained by excitation with left- and right-circulary polarized light. When solvent conditions of PIA-actin were changed by addition of NaCl, TFE, or ATP, ΔF showed sensitive responses to these compounds. From the analysis of ΔF_M and ΔF_E which represent the peaks of ΔF at the monomer- and excimer-emission band, the information concerned with the actin intrastructural changes were obtained. This method based on monitoring the excimer fluorescence with FDCD could be used for other proteins to extract finer structural changes that cannot be detected by the normal fluorescence spectroscopy.

（5） 荻野竜樹：**共通並列計算電磁流体・粒子コードによる太陽風磁気圏電離圏ダイナミックスの研究**，平成 14 年度～平成 17 年度科学研究費補助金（基盤研究（A））研究成果報告書（2006）

ABSTRACT：近年コンピュータシミュレーションを実行するスーパーコンピュータの環境が急速に変わってきた。それは，ベクトル並列機からスカラー並列機への移行である。国内でも，日立がベクトル並列機からスカラー並列機（Hitachi SR11000）へ移行して富士通もそれに続き（PRIMEPOWER HPC2500），2004 年度以降にベクトル並列機の開発を継続しているのは NEC のみ（NEC SX8）となった。こうした状況下，スペースプラズマ現象を効率よく並列計算できる，High PerformanceFortran（HPF）と Message Passing Interface（MPI）のコンピュータ言語を用いた共通並列電磁流体コード，粒子コード，及びハイブリッドコードを作成して，世界に先駆けた大規模シミュレーションを行い，スペースプラズマの非線形物理に新しい知見をもたらすのが本研究の目的であった。

領域分割法を導入し，ベクトル並列機に対しては HPF と MPI などいずれの並列化方法でも高効率の並列プログラムを作成することに成功した。優れた HPF コンパイラーが日本で独自に拡張・開発されたものの HPF の普及は結局伸びず，共通並列計算法としては MPI が残るのみとなった。一方，PRIMEPOWER HPC2500 などのスカラー並列機では，ベクトル並列機で高効率であった 1 次元領域分割の MPI3 次元 MHD コードは 100 個程度までの CPU 数まではほとんど変更無しで同程度の高速化を実現できたが，それを超えると並列化効率がほとんどよくならないことも判った。ここに，キャッシュのヒット率向上と 3 次元領域分割法の導入と一括データ転送を両立させた新しい MPI Fortran3 次元 MHD コードを開発することにより，スカラー並列機で高効率計算を実現する共通並列計算手法の確立に成功した。これらの手法は MPI Fortran が利用できれば広く応用できる方法である。その具体的な記述は名古屋大学情報連携基盤センターのニュース（解説）として公表するとともに，コンプリートプログラムを含めて，その最新の追加説明記述を含めて下記の Homepage で公開している。

（http://center.stelab.nagoya-u.ac.jp/kaken/kakenhi.html）

（6） Shoichiro IKEDA，*Kuranoshin KATO，and Osamu TSUKAMOTO：**Seasonal evolution of atmospheric and land surface conditions around the Huaihe River Basin in China in the pre-Meiyu stage of 1998**，OKAYAMA University Earth Science Reports，Vol.12，No.1，pp.31 ～ 37（2005）

ABSTRACT：Seasonal evolution of atmospheric and land surface conditions around the Huaihe River Basin in China in the pre-Meiyu stage of 1998 were examined, mainly based on the GAME re-analysis data. Around the Huaihe River Basin in China (just to the north of the Changjiang River Basin), although the air temperature increased rapidly already in early June (the Meuyu front was located to the south of that region), the specific humidity did not increase so much at that time. In addition, the latent heat supplied from the ground there decreased from late May to early June, compared to that before early May. The time mean southerly wind component across the low-level baroclinic zone (although not so strong as in the mature stage of the Meiyu) invaded into Central China during late April to early May. On the other hand, the relatively strong wind region once retreated southward in the middle of May associated with the onset of the Southeast Asian monsoon, and the calm wind region with frequent appearance of the surface high was seen around the Huaihe River Basin from late May to early June. Thus the present study shows that the Huaihe River Basin once experiences the rather drier stage just before the onset stage of the mature Meiyu there.

（7） 加藤晴子，＊加藤内藏進：**日本の春の季節進行と童謡・唱歌，芸術歌曲にみられる春の表現－気象と音楽の総合的な学習の開発に向けて－**，岡山大学教育実践総合センター紀要，第 6 巻，pp.39 ～ 54（2006）

ABSTRACT：学校教育では，教科の枠組みをこえた総合的な学習が注目されている。本研究では，気象と音楽を総合させた学習について考察した。気候や風土等の自然環境はその地域の音楽文化と深い関わりをもつ。したがって学校教育では，気象を視点として，気候などの自然環境と音楽作品の背景にある文化的要素を関連させた学習を行うことが可能であると考える。これまでの研究で，ドイツの春の気候と歌曲にみる春の表現の関係について明らかにしてきた。本研究では，日本の春の気候と歌の関係を取り上げて考察する。まず，日本の童謡・唱歌および芸術歌曲の中の春を歌った曲にみられる音楽表現について分析・検討を行い，次に春の表現と最も深く関係する季節進行過程について考察した。それらの考察結果をもとに，小学校と中学校における音楽と気象を総合させた学習プランを提示した。

（8） * 速水敏彦，木野和代，高木邦子：**他者軽視に基づく仮想的有能感－自尊感情との比較から－**，感情心理学研究，Vol.12，No.2，pp.43 ～ 55（2005）

ABSTRACT：It is said that adolescents nowadays are more likely to get angry. This phenomenon seems to be related to a kind of competence based on undervaluing others. Thus, a new construct "assumed-competence" is proposed in this study. The purpose of Study 1 is to formulate a new scale measuring the individual differences in assumed-competence and to examine the construct validity of the scale by mainly comparing it with self-esteem in relation to past experiences. Four scales designed to measure assumed-competence, past experiences, self-esteem, and narcissistic-competence were administered to 393 university students. It was found that ACS（Assumed-Competence Scale）consisting of 11 items had high reliability. It was not related to self-esteem at all, but positively related to narcissistic-competence. Self-esteem was positively correlated with positive experiences and assumed-competence was also positively correlated with negative experiences. Study 2 aims at investigating the relation between assumed-competence and anger which was measured using Spielberger's STAXI. It was evident that individuals with high assumed-competence had higher trait anger than those with low assumed-competence. Also, self-esteem inhibited the expression of anger.

（9） *Kunihiko Gekko，Yuichi Kunori，Hideatsu Takeuchi，Shigeyuki Ichihara，and Michiko Kodama：**Point Mutations at Glycine-121 of Escherichia coli Dihydrofolate Reductase:Important Roles of a Flexible Loop in the Stability and Function**，The Journal of Biochemistry，Vol.116，pp.34 ～ 41（1994）

ABSTRACT：To elucidate the role of a flexible loop in the stability and function of Escherichia coli dihydrofolate reductase, glycine-121 in a flexible loop（residues 117-131）, separated by 19 A from active site Asp27, was substituted by site-directed mutagenesis with eight amino acids（Ala, Val, Leu, Asp, Ser, Cys, Tyr, and His）. The free energy change of unfolding decreased in the order of G121A > G121D > G121C > G121S, wild-type > G121H > G121Y > G121L > G121V. The thermal denaturation temperature decreased with all mutations, accompanied by a decrease in the calorimetric enthalpy of denaturation. The steady-state kinetic parameter for the enzyme reaction, Km, was only slightly influenced, but kcat was significantly decreased by the mutations, there being 3-（G121C）to 42-fold（G121L）decreases in kcat/Km compared to that of the wild-type enzyme. The effects of mutations on the stability and enzyme activity were statistically examined as a function of the hydrophobicity and volume of amino acids introduced. The diminished stability and activity with increases in the hydrophobicity and volume of amino acids suggest that the main effect of the mutations would be

modification of the flexibility of the loop due to overcrowding of the bulky side chains, overcoming the enhancement of the hydrophobic interaction.

(10) Eiji Ohmae, Koji Iriyama, Shigeyuki Ichihara, and *Kunihiko Gekko : **Effects of Point Mutations at the Flexible Loop Glycine-67 of Escherichia coli Dihydrofolate Reductase on Its Stability and Function**, The Journal of Biochemistry, Vol.119, pp.703 ～ 710 (1996)

ABSTRACT : To elucidate the role of a flexible loop (residues 64-72) in the stability and function of Escherichia coli dihydrofolate reductase, glycine-67 in this loop was substituted by site-directed mutagenesis with seven amino acids (Ala, Cys, Asp, Leu, Ser, Thr, and Val). The circular dichroism spectra suggested that the confirmation of the native structure was affected by the mutations in both the presence and absence of NADPH. The free energy change of unfolding by urea decreased in the order of G67A > G67S > or = wild-type > or = G67D > G67T > G67C > or = G67L > G67V. The steady-state kinetic parameters for the enzyme reaction, Km and kcat, were only slightly influenced, but the rate of the hydride transfer reaction was significantly changed by the mutations, as revealed by the deuterium isotope effect on the enzyme activity. These results suggest that site 67 in the flexible loop, being very far from the active site, plays an important role in the stability and function of this enzyme. The characteristics of the mutations were discussed in terms of the modified flexibility of the native structure, compared with the results of mutations at site 121 in another flexible loop.

(11) Eiji Ohmae, Toshiyuki Kurumiya, Shio Makino, and *Kunihiko Gekko : **Acid and Thermal Unfolding of Escherichia coli Dihydrofolate Reductase**, The Journal of Biochemistry, Vol.120, pp.946 ～ 953 (1996)

ABSTRACT : The acid and thermal unfolding of Escherichia coli dihydrofolate reductase (DHFR) were studied by means of circular dichroism (CD) and fluorescence spectroscopy. There existed at least one intermediate around pH 4 in the acid unfolding process at 15 degrees C, in which the tertiary structure was disrupted before unfolding of the secondary structure. The fluorescence energy transfer from intrinsic tryptophan residues to 1-anilinonaphthalene-8-sulfonate suggested the disruption of the tertiary structure around some tryptophan residues of the intermediate. The thermal unfolding process at pH 7.0 also involved at least one intermediate having a disrupted tertiary structure and a folded secondary structure. The three-state thermodynamic analysis showed that the intermediate in thermal unfolding was less stable by 1.8 kcal/mol than the native state. The similarity of the far-ultraviolet CD spectra of acid and thermally

unfolded forms suggests that both types of unfolding produce the same structure, which may be a molten globule intermediate such as that in the folding kinetics of DHFR. The acid and thermal unfolding were depressed in the presence of KCl due to stabilization of the native form.

(12) Eiji Ohmae, Koji Iriyama, Shigeyuki Ichihara, and *Kunihiko Gekko : **Nonadditive Effects of Double Mutations at the Flexible Loops,Glycine-67 and Glycine-121,of Escherichia coli Dihydrofolate Reductase on Its Stability and Function**, The Journal of Biochemistry, Vol.123, pp.33 ～ 41 (1998)

ABSTRACT : The structure, stability, and enzymatic function of dihydrofolate reductase (DHFR) from Escherichia coli are influenced by point mutations at sites 67 and 121 in two flexible loops [Gekko et al. (1994) J. Biochem. 116, 34-41; Ohmae et al. (1996) J. Biochem. 119, 703-710]. In the present study, eight double mutants at sites 67 and 121 (G67V/G121S, G67V/G121A, G67V/G121C, G67V/G121D, G67V/G121V, G67V/G121H, G67V/G121L, and G67V/G121Y) were constructed in order to identify interactions between the two sites of DHFR. The far-ultraviolet circular dichroism spectra of double mutants were clearly different from those of the respective single mutants, with significant changes being observed for three mutants, G67V/G121A, G67V/G121L, and G67V/G121S. The Gibbs free energy change of urea unfolding of double mutants could not be expressed by the sum of those of the respective single mutants except for G67V/G121H. The steady-state kinetic experiments showed that the effect of double mutations manifests itself not in Km but in k (cat), and the transition-state stabilization energy for G67V/G121A, G67V/G121C, and G67V/G121L is not equal to the sum of those for the single mutants. These results indicate that the additivity rule essentially does not hold for these double mutants, and that long-range interactions occur between sites 67 and 121, even though they are separated by 27.7 A. This is evidence that the flexible loops play important roles in the stability and function of this enzyme through structural perturbations, in which a small alteration in local atomic packing due to amino acid substitution is cooperatively magnified over almost the whole molecule.

(13) Eiji Ohmae, Kenji Ishimura, Masahiro Iwakura, and *Kunihiko Gekko : **Effects of Point Mutations at the Flexible Loop Alanine-145 of Escherichia coli Dihydrofolate Reductase on Its Stability and Function**, The Journal of Biochemistry, Vol.123, pp.839 ～ 846 (1998)

ABSTRACT : To elucidate the role of a flexible loop (residues 142-149) in the stability and function of Escherichia coli dihydrofolate reductase, alanine-145 in this loop was

substituted by site-directed mutagenesis with ten amino acids (Glu, Phe, Gly, His, Ile, Leu, Arg, Ser, Thr, and Val). The amount of three mutant proteins (A145E, A145I, and A145L) in cells was too small to allow the measurement of circular dichroism (CD) spectra and urea unfolding. The CD spectra of other seven mutants were identical with those of the wild-type DHFR, indicating that the native conformation of DHFR was not affected by the mutations. The free energy change of unfolding by urea decreased with an increase in the hydrophobicity of amino acid residues introduced, A145T>A145R>A145G> or =A145S> or =A145H>A145V>wild-type> or =A145F. The steady-state kinetic parameters for the enzyme reaction, Km and ksub, were only slightly influenced by the mutations. These results suggest that site 145 in the flexible loop plays an important role in the stability but has little or no effect on the native structure and function of this enzyme. The characteristics of the mutations are discussed in comparison with those of mutations at site 67 [Ohmae et al. (1996) J. Biochem. 119, 703-710] and at site 121 [Gekko et al. (1994) J. Biochem. 116, 34-41] in two other flexible loops.

(14) Eiji Ohmae, Yoshie Sasaki, and *Kunihiko Gekko : **Effects of Five-Tryptophan Mutations on Structure,Stability and Function of Escherichia coli Dihydrofolate Reductase**, The Journal of Biochemistry, Vol.130, pp.439 ～ 447 (2001)

ABSTRACT : To elucidate the roles of tryptophan residues in the structure, stability, and function of Escherichia coli dihydrofolate reductase (DHFR), its five tryptophan residues were replaced by site-directed mutagenesis with leucine, phenylalanine or valine (W22F, W22L, W30L, W47L, W74F, W74L, W133F, and W133V). Far-ultraviolet circular dichroism (CD) spectra of these mutants reveal that exciton coupling between Trp47 and Trp74 strongly affects the peptide CD of wild-type DHFR, and that Trp133 also contributes appreciably. No additivity was observed in the contributions of individual tryptophan residues to the fluorescence spectrum of wild-type DHFR, Trp74 having a dominant effect. These single-tryptophan mutations induce large changes in the free energy of urea unfolding, which showed values of 1.79-7.14 kcal/mol, compared with the value for wild-type DHFR of 6.08 kcal/mol. Analysis of CD and fluorescence spectra suggests that thermal unfolding involves an intermediate with the native-like secondary structure, the disrupted Trp47-Trp74 exciton coupling, and the solvent-exposed Trp30 and Trp47 side chains. All the mutants except W22L (13%) retain more than 50% of the enzyme activity of wild-type DHFR. These results demonstrate that the five tryptophan residues of DHFR play important roles in its structure and stability but do not crucially affect its enzymatic function.

（15） 木方十根：**戦前期東京における高等教育機関キャンパスの形成段階と分布形態**，日本都市計画学会学術研究論文集，No.35，pp.139 ～ 144（2000）

（16）*村田健史，ヌルディヤナ B.A. ガーニ，橋本弘蔵，松本紘，荻野龍樹：**バーチャル地球磁気圏システムの提案**, 電子情報通信学会論文誌 B, Vol.J87-B, No.2, pp.309 ～ 313（2004）

（17） 小平英志：**理想自己と義務自己の内在状態の差異―現実自己の参照度および関連付けられるエピソード―**，名古屋大学大学院教育発達科学研究科紀要（心理発達科学），Vol.51，pp.99 ～ 105（2004）

ABSTRACT：This study investigated the differences between the ought selves and the ideal selves in relationship to actual selves and accessing episodes. Participants（N=157）were asked to describe ideal selves and ought selves, the reason to desires such, and the time and the occurrence which began to be conscious. Frequencies in which the actual selves appeared as reason, and of positive/negative episode related each self-guide were counted. Results showed that the ought selves were not linked to the actual selves rather than the ideal selves. But there was no significant difference between the ideal selves and the ought selves in episode（negative/positive）related to self-guides. These results suggested the obsessive aspect of ought selves and integration of ideal selves and ought selves.

（18） Masaki Ogawa：**Chemical stratification in a two-dimensional convecting mantle with magmatism and moving plates**，JOURNAL OF GEOPHYSICAL RESEARCH, Vol.108，No.B12，pp.ETG5-1 ～ 20（2003）

ABSTRACT：A self-consistent numerical model is presented for magmatism in a convecting mantle with moving plates. Mantle convection is modeled as a thermal-chemical convection of binary eutectic material with Newtonian rheology in a two-dimensional rectangular box internally heated by incompatible radioactive elements. Viscosity is assumed to depend on stress-history as well as temperature and pressure to self-consistently reproduce moving plates. The solid-solid phase transitions at depths around 660 km, which work as a partial barrier to convective flow across the 660 km phase boundary, are also taken into account. Magmatism is modeled as a permeable flow of basaltic melt produced upon decompression melting of the convecting material through the coexisting matrix. Magmatism makes mantle chemically stratified with the shallower part occupied by chemically buoyant residue of magma depleted in radioactive elements and the deeper part occupied by hot but chemically dense materials enriched in basaltic component and radioactive elements even under the influence of moving plates

and subducting slabs. The magmatism is induced by moving plates (ridge volcanism), mantle overturn, and hot plumes uprising from the 660 km phase boundary or the lower mantle, depending upon the internal heating rate and the strength of the 660 km barrier to the convective flow across the phase boundary. When plates move, subducting slabs penetrate deep into the lower mantle and induce broad thermal and chemical heterogeneity at depth in the lower mantle. The chemically stratified mantle with moving plates is compared to the earth's mantle.

(19) *T.Sugiyama, M.Fujimoto, H.Matsumoto : **Energy Spectra of Energetic Ions Around Quasi-Parallel Shocks**, AGUs Geophysical Monograph series of "Astrophysical Particle Acceleration in Geospace and Beyond", Vol. 156, pp.87 ～ 95 (2005)

ABSTRACT : We have performed a number of simulations of quasi-parallel shocks to investigate how the energy spectra of non-thermal components are controlled by the presence of alpha (He2+) particles. The simulations are done for the Earth's bow shock-like situation by an one-dimensional hybrid code that treats ions as particles but electrons as a massless fluid. The upstream conditions are modified by varying the He2+ ions content while keeping the proton content unchanged. The range of the He2+ ion density ratio (R) variation relative to proton is from 0.1 % to 30 % including the typical ratio of 4 ～ 5 % for the solar wind. As observed in the upstream of the bow shock, the differential flux spectra of the two ion species obtained in the simulations from the downstream region are found to be well represented by exponential shapes. When the energy scale is presented in the energy-per-charge (E/Q) unit, the two spectra have the same characteristic energy (Ec) that increases in time. While Ec is a function of the density ratio R and increases with increasing R, the equality between the two species holds throughout. Detailed analyses show that larger magnetic fluctuations brought about by the presence of He2+ particles enable more efficient acceleration at the shock front. Thus it is via exciting, stronger turbulence that the additional upstream ram energy carried by He2+ ions is poured into the process of hardening the energy spectrum of the non-thermal particles of both species.

(20) Kazutomo Kawaguchi, *Takahisa Yamato : **Theoretical prediction of optical absorption maxima for photosensory receptor mutants**, Chemical Physics Letters, Vol.430, pp.386 ～ 390 (2006)

ABSTRACT : We found a linear correlation between the theoretically predicted shifts and experimentally observed absorption spectra for various mutants of photoactive yellow

protein（PYP）, a photosensory receptor. Excitation energies of mutants were evaluated by the combination of the high level ab initio calculation for the chromophore inside and the low level ab initio calculation for the surrounding protein environment. Importantly, the electronic states of these two regions were treated both as variables and they are solved consistently to each other. The protein-chromophore interaction has been accurately reproduced by this method.

（21） Takakazu Ishikura, *Takahisa Yamato：**Energy transfer pathways relevant for long-range intramolecular signaling of photosensory protein revealed by microscopic energy conductivity analysis**, Chemical Physics Letters, Vol.432, pp.533 ～ 537（2006）

ABSTRACT：We report a theoretical/ computational analysis of the energy flow relevant to the long-range intramolecular crosstalk between different regions in a photosensory receptor, photoactive yellow protein（PYP）. To analyze the energy flow in atomic detail, we derived a theoretical expression for the interresidue energy conductivity in terms of the time-correlation function of the interatomic energy flux. The values of energy conductivities were numerically evaluated by using a long molecular dynamics simulation trajectory of the PYP molecule in the aqueous solution environment. As a result, we detected several pathways for energy transfer relevant for the long-range intramolecular signalling of PYP.

（22） *S.Zenitani and M.Hoshino：**Three-Dimensional Evolution of a Relativistic Current Sheet:Triggering of Magnetic Reconnection by the Guide Field**, PHYSICAL REVIEW LETTERS, Vol.95, 095001-1 ～ 4（2005）

ABSTRACT：The linear and nonlinear evolution of a relativistic current sheet of pair plasmas is investigated by three-dimensional particle-in-cell simulations. In a Harris configuration, it is obtained that the magnetic energy is fast dissipated by the relativistic drift kink instability（RDKI）. However, when a current-aligned magnetic field（the so-called "guide field"）is introduced, the RDKI is stabilized by the magnetic tension force and it separates into two obliquely propagating modes, which we call the relativistic drift-kink-tearing instability. These two waves deform the current sheet so that they trigger relativistic magnetic reconnection at a crossover thinning point. Since relativistic reconnection produces a lot of nonthermal particles, the guide field is of critical importance to study the energetics of a relativistic current sheet.

（23） *Shinichi Murayama, Toru Mori, and Koichi Nishigaki：**CORRELATION BETWEEN THE HELIX-FORMING PROPENSITY OF PEPTIDES OBTAINED**

BY NS MD SIMULATION AND THE Chou-Fasman PARAMETERS, BIOINFO 2005 Proceedings of the 2005 International Joint Conference of InCoB,AASBi and KSBI (2005)

ABSTRACT：Molecular dynamics of nanosecond timescale could provide a significant result for the structure analysis of oligopeptides. The most surprising was the fact that Chou-Fasman parameters which have no direct relationship with nanosecond molecular dynamics could implicate the result to a certain extent. A novel parameter termed X % -stickiness, which is another measure of compactness of a molecule, was first introduced successfully.

(24) * 村山真一，吉田昼也，青山崇，浦田賢，西垣功一：**ナノ秒の MD シミュレーションから求めたペプチド二次構造の確率予測－三角マップ表示した％スティッキネス法の有用性**，Journal of Computer Chemistry, Japan，Vol.5，No.4，pp.213 ～ 218（2006）

ABSTRACT：ペプチドのナノ秒（ns）分子動力学計算（MD）では，安定構造を得るのには遙かに不十分な計算時間であることが分かっている。にもかかわらず，新たに導入した％スティッキネスの三角マップ表示（TMR-％σ）によって，安定構造に含まれる二次構造（特にα ヘリックス）のおぼろげな像が得られることが示された。％スティッキネスとは，生体高分子の動的なコンフォメーション変化を記述する目的で以前に導入された指標である。TMR-％σ 表示において，ペプチド形成傾向は，マップ上にα ヘリックス固有の相互作用を示すシフトした対角線ラインとして現れた。ns-MD の結果から計算されたペプチドの％σ と旋回半径（Rg）の座標プロットから，ペプチドの二次構造予測に関する確率マトリクスを導出できることが示された。

(25) *Yoshimitsu Niwa，Hiroshi Yatsuya，Koji Tamakoshi，Kazuko Nishio，Takaaki Kondo，Yingsong Lin，Sadao Suzuki，Kenji Wakai，Shinkan Tokudome，Akio Yamamoto，Nobuyuki Hamajima，Hideaki Toyoshima，and Akiko Tamakoshi for the JACC Study Group：**Relationship between body mass index and the risk of ovarian cancer in the Japanese population:Findings from the Japanese Collaborate Cohort（JACC）study**，The Journal of Obstetrics and Gynaecology Research，Vol.31，No.5，pp.452 ～ 458（2005）

ABSTRACT：【目的】日本における卵巣癌罹患は 1970 年代以降増加している。文部科学省の助成する大規模コホート研究（The JACC study）のデータを用いて，日本人女性における body mass index（BMI）と卵巣癌罹患リスクの関連性について検討を行った。【方法】1988-1990 年より 40-79 歳の女性を対象に追跡調査を行った。研究開始時に，自記式調査票により生活習慣の情報を収集した。罹患調査地区の 36,456 人を解析対象とした。平均 7.6 年の追跡期間で，解析対象者における卵巣癌罹患は 38 例であった。

Cox 比例ハザードモデルを用いて，年齢，家族歴，生殖歴，喫煙習慣などの交絡要因を調整した相対危険度と 95％信頼区間を計算した。

【結果】卵巣癌罹患の相対危険度は BMI=18.5-24.9 kg/m^2 の女性に比べて BMI<18.5 kg/m^2，BMI=25.0-29.9 kg/m^2，BMI<30.0 kg/m^2 の女性の卵巣癌罹患の相対危険度はそれぞれ 0.43（95％信頼区間：0.06-3.18），2.24（95％信頼区間：1.10-4.21），1.78（95％信頼区間：0.24-13.34）であった。

【総括】日本人女性において，BMI の増加は卵巣癌のリスクファクターである可能性が示された。