

■研究成果の発表実績（学会、論文、その他啓発活動等/2025 年度）

課題名	研究成果の発表実績
課題 1	SCA/HPC Asia 2026, Osaka, Jan 26-29, 2026 AI-Drug Discovery Platform KOBE として COE 課題に関する成果をスライドで報告
課題 2	・Tristan Hascoet, Victor Pellet, Satoru Oishi, Takemasa Miyosh, 2026: Differentiable River Routing for End-to-End Learning of Hydrological Processes, JGResearch: Machine Learning and Computation, 3(1), e2025JH000760 ・足立幸穂, 河合佑太, 西澤誠也, 岡崎淳史, 佐藤陽祐, 新田友子, 2025: 気象気候モデル SCALE の紹介と陸面モデル MATSIRO の導入. 気候変動適応の研究会, 東京 ・Mizuki Funato, Fukuharu Tanaka, Hirozumi Yamaguchi, Agent-Based Modeling of Flood Evacuation Dynamics Driven by Large Language Models, SCAsia2026 Poster, P-161 ・Fukuharu Tanaka, Hamada Rizk, Hirozumi Yamaguchi, Global Indoor Positioning Powered by a Supercomputing-Driven Architecture, SCAsia2026 Poster, P-234 ・Hibiki Yoshizaki, Akira Uchiyama, Akihito Hiromori, Mineo Takai and Hirozumi Yamaguchi , A Lightweight Vision-Language Model for Disaster Image Summarization, Proceedings of the 5th Workshop on Pervasive and Resource-Constrained Artificial Intelligence (PerconAI 2026), pp. 1203-1208, 2026 ・Fukuharu Tanaka, Takamasa Higuchi, Masaki Takanashi, Tatsuya Amano, Hamada Rizk, Akira Uchiyama, Akihito Hiromori and Hirozumi Yamaguchi, On the Impact of Terrain Types in Deep Neural Network-Based Surrogates of Radio Maps, Proceedings of the 15th International Conference on Mobile Computing and Ubiquitous Networking (ICMU2025), pp. 1-6, 2025 ・Yu Yasuda, Tatsuya Amano and Hirozumi Yamaguchi, A Digital Twin Approach for Crowd Flow Modeling on Railway Station Platforms, Proceedings of the 2025 IEEE International Conference on Smart Computing (SmartComp2025), pp. 82-89, 2025 ・天野 辰哉, 山口 弘純, 実データ同化型シミュレーションに向けた大規模言語モデルによる観光客行動の予測手法, 人工知能学会第 1 回計算創律科学研究会, Vol. CSS-001, pp. 34-40, 2025 ・矢野 敦大, 天野 辰哉, 山口 弘純, 先見シミュレーションに非同期観測を同化する人流デジタルツイン, 情報処理学会研究報告 (情処技報), Vol. 2025-ITS-103, Vol. 25, pp. 46030, 2025 ・矢野 敦大, 天野 辰哉, 山口 弘純, 大規模人流デジタルツインに基づく屋内移動計画支援システムの設計と開発, マルチメディア, 分散, 協調とモバイルシンポジウム 2025 論文集, pp. 1137-1144, 2025
課題 3	【論文】 1. Kazuya Shinjo, Kazuhiro Seki, Tomonori Shirakawa, Rong-Yang Sun, Seiji Yunoki, “Unveiling clean two-dimensional discrete time crystals on a digital quantum computer”, npj Quantum Information 12, 41 (2026) [DOI: 10.1038/s41534-026-01193-3] 2. Satoshi Ejima, Kazuhiro Seki, Benedikt Fauseweh, Seiji Yunoki, “Probabilistic imaginary-time evolution in state-vector-based and shot-based simulations and on quantum devices”, Phys. Rev. Research 7, 043182 (2025) [DOI: 10.1103/2s2p-kvcx] 3. Han Xu, Kazuhiro Seki, and Seiji Yunoki, “Preparing the Gutzwiller wave function for attractive SU(3) fermions on a quantum computer”, Phys. Rev. Research 7, 033290 (2025) [DOI: 10.1103/rc6z-837q]

4. Yuichi Otsuka, Kazuhiro Seki, and Seiji Yunoki, “Quantum conditional mutual information as a probe of measurement-induced entanglement phase transition”, *Phys. Rev. B* **112**, 054301 (2025) [DOI: 10.1103/th2c-pdpw]
5. Kazuya Shinjo, Shigetoshi Sota, Seiji Yunoki, and Takami Tohyama, “Optical absorption activated by an ultrashort half-cycle pulse in metallic and superconducting states of the Hubbard model”, *Phys. Rev. B* **111**, 235125 (2025) [DOI: 10.1103/qlfw-tdkl]
6. Kazuhiro Seki, Yuta Kikuchi, Tomoya Hayata, Seiji Yunoki, “Simulating Floquet scrambling circuits on trapped-ion quantum computers”, *Phys. Rev. Research* **7**, 023032 (2025) [DOI: 10.1103/PhysRevResearch.7.023032]
7. Javier Robledo-Moreno, Mario Motta, Holger Haas, Petar Jurcevic, William Kirby, Simon Martiel, Kunal Sharma, Sadeep Sharma, Tomonori Shirakawa, Iskandar Sitdikov, Rong-Yang Sun, Kevin J. Sung, Maika Takita, Minh C. Tran, Seiji Yunoki, Antonio Mezzacapo, “Chemistry beyond the scale of exact diagonalization on a quantum-centric supercomputer”, *Science Advances* **11**, adu9991 (2025) [DOI: 10.1126/sciadv.adu9991]
8. Ryo Watanabe, Hidetaka Manabe, Toshiya Hikiyara, Hiroshi Ueda, “TTNOpt: Tree tensor network package for high-rank tensor compression”, *Computer Physics Communications* **319**, 109918 (2026) [DOI: 10.1016/j.cpc.2025.109918]
9. Takumi Kaneda, Keisuke Fujii, Hiroshi Ueda, “Large-scale quantum device benchmarking via LXEB with particle-number-conserving random quantum circuits”, *Physical Review Research* **8**, 013082 (2026) [DOI: 10.1103/ssrm-kddv]
10. Toshiya Hikiyara, Hiroshi Ueda, Kouichi Okunishi, Kenji Harada, Tomotoshi Nishino, “Improving the accuracy of the tree-tensor network approach by optimization of network structure”, *Physical Review B* **112**, 134427 (2025). [DOI: 10.1103/ljj8-tkpc]
11. Maxence Vandromme, Miwako Tsuji, “Post-Variational Quantum Neural Networks on a Hybrid HPC-QC System”, *Proceedings of the SC ’25 Workshops of the International Conference for High Performance Computing, Networking, Storage and Analysis*, 1816, (2025) [DOI: 10.1145/3731599.3767540]
12. Soratouch Pornmaneerattanatri, Miwako Tsuji, Mitsuhsa Sato, Ketan Maheshwari, “Python-based Workflow System for Quantum-HPC Hybrid Application on HPC System and Quantum Computer with Shared Network”, *SCA/HPCAsiaWS ’26: Proceedings of the Supercomputing Asia and International Conference on High Performance Computing in Asia Pacific Region Workshops*, 428, (2026) [DOI: 10.1145/3784828.3786263]
13. Gilles Buchs, Thomas L. Beck, Ryan S. Bennink, Daniel Claudino, rea Delgado, Nur Aiman Fadel, Peter Groszkowski, Kathleen E. Hamilton, Travis S. Humble, Neeraj Kumar, Ang Li, Phillip C. Lotshaw, Olli Mukkula, Ryousei Takano, Amit Saxena, In-Saeng Suh, Miwako Tsuji, Roel Van Beeumen, Ugo Varetto, Yan Wang, Kazuya Yamazaki, Mikael P. Johansson, “The Role of Quantum Computing indvancing Scientific High-Performance Computing: perspective from the ADAC Institute”, *Future Generation Computer Systems* **182**, 108487, (2026) [DOI: 10.1016/j.future.2026.108487]
14. Brice Chichereau, Stephane Vialle, Miwako Tsuji, Patrick Carribault, Mitsuhsa Sato, “HPCQCMARK: a new modular HPC-QC benchmarking framework”, *2025 IEEE International Conference on Quantum Computing and Engineering (QCE)*, **8** (2025) [DOI: 10.1109/QCE65121.2025.10285]
15. Matthias Brosz, Johanna Buck, Fabian Grünewald, Debora Monego, Jaewoon Jung, Yuji Sugita, Camilo Aponte-Santamaría, Frauke Gräter, “Coarse-grained Martini 3 model for collagen fibrils”, *Biophys. J.* **20**, 581 (2026) [DOI: 10.1016/j.bpj.2025.10.012]
16. Diego Ugarte La Torre, Yuji Sugita, “CGBack: Diffusion Model for Backmapping Large-Scale and Complex Coarse-Grained Molecular Systems”, *J. Chem. Inf. Model* **65**, 9974 (2025) [DOI: 10.1021/acs.jcim.5c01281]

17. Daisuke Matsuoka, Yuji Sugita, Takaharu Mori, “An Empirical Biasing Force Constant to Minimize Overfitting in Cryo-EM Flexible Fitting Refinement”, *J. Chem. Inf. Model.* 65, 18, 9790 (2025) [DOI: 10.1021/acs.jcim.5c01424]
18. Masahiro Motohashi, Mao Oide, Chigusa Kobayashi, Jaewoon Jung, Eiro Muneyuki, Yuji Sugita, “The distortion–push mechanism for the γ subunit rotation in F1-ATPase”, *Proc. Natl. Acad. Sci. USA* 122, e2502642122 (2025) [DOI: 10.1073/pnas.2502642122]
19. Debora Monego, Matthias Brosz, Johanna Buck, Vsevolod Viliuga, Paulius Greicius, Jaewoon Jung, Torsten Stuehn, Matthias Schmies, Yuji Sugita, Frauke Gräter, “ColBuilder: Flexible structure generation of crosslinked collagen fibrils”, *Bioinformatics* (2025), btaf278 [DOI: 10.1093/bioinformatics/btaf278]
20. Soundhararajan Gopi, Giovanni B Brandani, Cheng Tan, Jaewoon Jung, Chenyang Gu, Azuki Mizutani, Hiroshi Ochiai, Yuji Sugita, Shoji Takada, “In silico nanoscope to study the interplay of genome organization and transcription regulation”, *Nucleic Acids Research* 53, gkaf189 (2025) [DOI: 10.1093/nar/gkaf189]
21. Azuki Mizutani, Cheng Tan, Yuji Sugita, Shoji Takada, “Heterogeneous condensates of transcription factors in embryonic stem cells: Molecular simulations”, *Biophysical Journal* 124, 1587 (2025) [10.1016/j.bpj.2025.04.001]
22. Kiyoshi Yagi, Klaas Gunst, Toru Shiozaki, Yuji Sugita, “High-performance QM/MM Enhanced Sampling Molecular Dynamics Simulations with GENESIS SPDYN and QSimulate-QM”, *J. Chem. Theory Comp.* 21, 8, 4016–4029 (2025) [DOI: 10.1021/acs.jctc.5c00163]
23. Rommie E Amaro et al. (including Yuji Sugita), “The need to implement FAIR principles in biomolecular simulations”, *Nature Methods* 22, 641(2025) [DOI: 10.1038/s41592-025-02635-0]
24. Ai Niitsu, Andrew R Thomson, Alistair J Scott, Jason T Sengel, Jaewoon Jung, Kozhinjampara R Mahendran, Mikiko Sodeoka, Hagan Bayley, Yuji Sugita, Derek N Woolfson, Mark I Wallace, “Rational Design Principles for De Novo α -Helical Peptide Barrels with Dynamic Conductive Channels”, *J. Am. Chem. Soc.* 147, 11741 (2025) [DOI: 10.1021/jacs.4c13933]
25. Jaewoon Jung, Yuji Sugita, “Langevin integration for isothermal–isobaric condition with a large time step”, *J. Chem. Phys.* 162, 104108 (2025) [DOI: 10.1063/5.0251642]
26. Yao-Kun Lei, Kiyoshi Yagi, Yuji Sugita, “Efficient Training of Neural Network Potentials for Chemical and Enzymatic Reactions by Continual Learning”, *J. Chem. Theory Comp.* 21, 5, 2695 (2025) [DOI: 10.1021/acs.jctc.4c01393]
27. Ai Niitsu, Jaewoon Jung, Yuji Sugita, “Structural dynamics of a designed peptide pore under an external electric field”, *Biophys. Chem.* 318, 107380 (2025) [DOI: 10.1016/j.bpc.2024.107380]

【総説】

1. Shingo Ito, Chigusa Kobayashi, Kiyoshi Yagi, Yuji Sugita, “Toward understanding whole enzymatic reaction cycles using multi-scale molecular simulations”, *Curr. Opin. Struct. Biol.* 95, 103153 (2025) [DOI: 10.1016/j.sbi.2025.103153]
2. Yuji Sugita, Robert Woods, “Editorial overview: Toward cellular-scale modeling: Bigger and disordered”, *Curr. Opin. Struct. Biol.* 93, 103121 (2025) [DOI: 10.1016/j.sbi.2025.103121]

【解説記事】

1. 白川知功, 柚木清司, “テンソルネットワーク法を用いた量子回路シミュレーション”, *日本シミュレーション学会「シミュレーション」* 44, 18–23 (2025)

【プレプリント】

1. Kentaro Yamamoto, Riku Masui, Takahito Nakajima, Miwako Tsuji, Mitsuhsa Sato, Peter Schow, Lukas Heidemann, Matthew Burke, Philipp Seitz, Oliver J. Backhouse, Juan W. Pedersen, John Children, Craig Holliman, Nathan Lysne, Daichi Okuno, Seyon Sivarajah, David Munoz Ramo, Alex Chernoguzov, Ross Duncan, “Quantum-HPC hybrid computation of biomolecular excited-state energies”, arXiv:2601.15677 (2026) [DOI: 10.48550/arXiv.2601.15677]
2. Ryo Watanabe, Joseph Tindall, Shohei Miyakoshi, Hiroshi Ueda, “Quantum-Inspired Algorithm for Classical Spin Hamiltonians Based on Matrix Product Operators”, arXiv:2602.05224 (2026) [10.48550/arXiv.2602.05224]
3. Ryo Watanabe, Toshiya Hikihara, Hiroshi Ueda, “Site-Order Optimization in the Density Matrix Renormalization Group via Multi-Site Rearrangement”, arXiv:2512.22021 (2025) [DOI: 10.48550/arXiv.2512.22021]

【講演・口頭発表など】

1. 白川知功, “量子 HPC 連携システムを使った量子多体シミュレーション”, 第3回 TN の媒介する量子・古典融合研究集会, AP イノゲート大阪, 大阪, 2026 年 3 月 30 日 [Invited]
2. Seiji Yunoki, “Towards quantum advantage in many-body physics via quantum-HPC hybrid computation”, APS Global Physics Summit 2026, Denver, USA, (March 18, 2026) [Invited]
3. Tomonori Shirakawa et al., “Large-Scale Quantum Chemistry Computations Using Quantum-HPC Hybrid Systems”, APS Global Physics Summit 2026, Denver, USA, (March 17, 2026)
4. Tomonori Shirakawa, “Quantum-HPC Application Development for Quantum Many-Body Systems: Selected_Basis Diagonalization and Tensor-Network Approach”, The 14th “FugakuNEXT” Application Seminar, online, (February 26, 2026)
5. 白川知功, “量子コンピュータとスーパーコンピュータの連携による 量子化学計算の高度化と産業応用の展望”, 川崎市・先端技術活用支援講座(量子セミナー)「量子計算の実装と高速化技術の現在地」、新川崎・創造のもり AIRBIC、(2026 年 2 月 20 日) [Requested]
6. Tomonori Shirakawa, “Utilizing quantum selected basis methods and tensor network techniques for quantum-HPC hybrid computing”, Seminar of Quantum Embedding Group in SQAI, online (January 19, 2026)
7. Tomonori Shirakawa, “Quantum Many-Body Computations on a Quantum-HPC Hybrid Platform”, The 1st Joint General Meeting of RIKEN Quantum and the QII RIKEN User Group, Wako, Japan (October 24, 2025)
8. Seiji Yunoki, “Prethermal time crystalline phases and noise-induced dynamics on digital quantum computers”, The 16th Asia Pacific Physics Conference, Haikou, China (October 19–24, 2025) [Invited]
9. Yuichi Otsuka, “Measurement-induced phase transition in variable-range random Clifford circuits”, Progress Report on R&D Topic 02, 6th SQAI General Meeting, Kobe, Japan (September 29, 2025)
10. Tomonori Shirakawa, “Quantum-HPC Hybrid Simulation for Quantum Chemistry”, SQAI-NCTS Workshop on Quantum Technologies and Machine Learning, Taipei, Taiwan (August 25–29, 2025) [Invited]
11. Seiji Yunoki, “Prethermal time crystalline phases and noise-induced dynamics on digital quantum computers”, SQAI-NCTS Workshop on Quantum Technologies and Machine Learning, Taipei, Taiwan (August 25–29, 2025) [Invited]
12. Tomonori Shirakawa, “Pushing the frontier of quantum-centric supercomputing for electronic structure calculations”, Materials Science Working Group In-Person Workshop 2025, Kobe, Japan (August 18–20, 2025)

13. Tomonori Shirakawa, “Quantum Chemistry on Quantum-HPC Hybrid Systems”, SQAI Summer Camp, Gunma (August 6-8, 2025)
14. Tomonori Shirakawa, “Quantum-HPC hybrid computing for Quantum Many-Body Problems”, Tensor Network 2025, Tokyo, Japan (July 16-18, 2025) [Invited]
15. Seiji Yunoki, “Quantum many-body dynamics simulations using digital quantum computers”, Joint International Workshop on Quantum Computing, Tainan, Taiwan (June 23-25, 2025) [Invited]
16. Seiji Yunoki, “Quantum many-body dynamics simulations using trapped-ion quantum computers”, The 2nd Workshop on Quantum Computation meets Quantum Many-Body Computation, Shanghai, China (June 17-20, 2025) [Invited]
17. Seiji Yunoki, “Pushing the frontier of quantum-centric supercomputing for electronic structure calculations”, IBM Quantum Partner Forum 2025, London (June 4-6, 2025) [Invited]
18. Seiji Yunoki, “Quantum many-body simulations using Quantinuum H1 systems”, Quantinuum May 2025 Training Session, Osaka, (May 19, 2025). [Invited]
19. Seiji Yunoki and Netanel Lindner, “Quantum-Enhanced HPC Simulations with Error Mitigation” (Plenary Talk), Q2B25 Tokyo (May 15-16, 2025) [Invited]
20. 上田宏, “DMRGにおけるサイト順序最適化手法の高度化”, 第3回 TNの媒介する量子・古典融合研究集会, イノゲート大阪, (2026年3月30日)
21. Hiroshi Ueda, “From Vector Data to Quantum Circuits: TTN0pt for Efficient Tensor-Network Encoding”, TNSAA2025, Tainan, (December 16, 2025) [Invited]
22. 上田宏, “量子多体計算から眺める量子コンピュータとAI”, PCCC25 (設立25年記念PCクラスタシンポジウム) 「HPC最前線」, 富士ソフト アキバプラザ, (2025年12月9日) [invited]
23. 佐藤三久, 上田宏, 高野了成, 辻美和子, 寺師弘二, “パネル討議: HPC、量子、AIの融合のビジョン”, PCCC25 (設立25年記念PCクラスタシンポジウム) 「HPC最前線」, 富士ソフト アキバプラザ, (2025年12月9日) [Invited]
24. 上田宏, “量子HPC連携プラットフォームの構築: 量子HPC連携の可能性と応用 一次世代計算の展望”, 次世代コンピューティングのフロンティア ~理化学研究所が取り組む計算可能領域の拡張~, CEATEC 2025, 幕張メッセ, (2025年10月16日) [Invited]
25. 渡辺亮, 真鍋秀隆, 引原俊哉, 上田宏, “TTN0pt: 高次元テンソル圧縮のためのツリーテンソルネットワークパッケージ”, 日本物理学会第80回年次大会, 広島大学, (2025年9月17日)
26. S. Miyakoshi, T. Sugimoto, H. Ueda, “Advancing Quantum Circuit Optimization Through Density Matrix Renormalization Group Techniques”, LT30, Bilbao, Spain, (August 12, 2025)
27. S. Miyakoshi, T. Sugimoto, H. Ueda, “Variational Quantum Circuit Optimization via Density Matrix Renormalization Group”, Quantum Innovation 2025, Osaka, (July 29, 2025) [Poster]
28. S. Miyakoshi, T. Sugimoto, H. Ueda, “Layered Quantum Circuit Construction Inspired by Density Matrix Renormalization Group”, StatPhys29, Florence, Italy, (July 14, 2025) [Poster]
29. S. Miyakoshi, T. Sugimoto, H. Ueda, “Density Matrix Renormalization Group-Inspired Framework for Efficient Quantum Circuit Optimization”, SCES2025, Montréal, Canada, (July 10, 2025).
30. Hiroshi Ueda, “Application of Tensor Network Schemes In Quantum Algorithms for Analyzing Many-Body Systems”, Quantinuum May 2025 Training Session, Osaka, (May 20, 2025) [Invited]
31. 辻美和子, 佐藤三久, “量子HPC連携プラットフォームに向けたソフトウェアとプログラミング環境”, 第255回システム・アーキテクチャ・第202回ハイパフォーマンส์コンピューティング合同研究発表会, 2025-HPC-202(14), pp.1-7, (2025年12月15日).
32. Miwako Tsuji, “量子HPC連携プラットフォームに向けたソフトウェア開発”, PCCC25 (設立25年記念PCクラスタシンポジウム) 「HPC最前線」, 東京, (2025年12月9日) [Invited]

	33. Miwako Tsuji, “Practice and Experience in JHPC-Quantum: HPC Oriented quantum-HPC integration”, QUEST-IS 2025, 1st International Quantum Engineering conference and exhibition, (December 4, 2025) [Invited] 34. Maxence Vandromme, Miwako Tsuji, Tatsuhiko Tsunoda, Lysenko Artem, Mitsuhisa Sato, “Visualizing the Effects of Quantum Circuits in a Hybrid Classical-Quantum Machine Learning Algorithm”, 第15回量子ソフトウェア研究発表会, 東京, (2025年6月26日) 35. 中嶋隆人, “量子古典ハイブリッド計算のための量子化学”, JHPC-quantum シンポジウム 2025, 東京, (2025年12月12日) 36. Hirofumi Tomita, “Redesign of the Next-Generation Dynamical Core Toward the Era of AI and Quantum Computing”, HANAMI High Level Symposium, Chamonix, France, (December 9, 2025) [Invited] 37. Yuji Sugita, “How are enzyme reactions activated in cellular crowding environments?”, Pachifichem Symposium on Biomolecules at Interfaces Defining the Cellular Environment: From Conformational Dynamics to Informatic Approaches, Hawaii, USA, (December 15-20, 2025) [Invited] 38. Yuji Sugita, “Efficient dimensional reduction methods for the free-energy landscapes of protein dynamics”, Pachifichem Symposium on Emerging Frontiers: Machine Learning Transforming Studies of Biomolecular Dynamics, Hawaii, USA, (December 15-20, 2025) [Invited] 39. Yuji Sugita, Development of enhanced conformational sampling methods for free-energy calculations of membrane proteins, Pachifichem Symposium on Crossing the Biological Membrane: Frontiers in the Study of Membrane Transport, Hawaii, USA, (December 15-20, 2025) [Invited] 40. Yuji Sugita, “Multi-Scale Molecular Dynamics Simulations of Biomolecules and Materials”, MRM2025, Yokohama, Japan, (December 8-13, 2025) [Invited] 41. Yuji Sugita, “The gamma subunit rotation in F1-ATPase with atomistic molecular dynamics simulations”, The 10th iHuman Forum, Shanghai, China, (October 2025) [Invited] 42. Yuji Sugita, “Multi-scale simulations of biomolecular condensate regulations”, SMART symposium, Shenzhen, China, (October 31, 2025) [Invited] 43. Yuji Sugita, “Integrated enhanced conformational sampling methods for biomolecular dynamics and functions”, CECAM Workshop: When data science meets molecular dynamics, Lausanne, Switzerland, (October 15-17, 2025) [Invited] 44. Yuji Sugita, “The Distortion-Push Mechanism for the g subunit rotation in F1-ATPase”, Tenth Polish-Korean Conference on “Protein Folding: Theoretical and Experimental Approaches”, Gdansk, Poland, (September 8-10, 2025) [Invited] 45. Yuji Sugita, “The rotation mechanisms of F1-ATPase using atomistic molecular dynamics simulations”, 2025 Hong Kong Symposium on Molecular Modeling and Simulation, Hong Kong, (May 23-26, 2025) [Invited] 46. Yuji Sugita, “How to regulate protein condensation with highly charged HERO proteins”, 2025 GCSC Symposium: Chemical Dynamics in Materials and Living Systems, Seoul, Korea, (May 6-10, 2025) [Invited]
課題4	<u>Publications</u> 1. Zhao, W., Miyashita, O. & Tama, F. xspline3d: A Python Library for MPI-Based Spline Interpolation Enforcing Global Continuity in Distributed 3D Volumes. Proc. Supercomputing Asia Int. Conf. High Perform. Comput. Asia Pacific Reg. Workshops 1-25 (2026).

2. Kanaoka, Y., Hamaguchi-Suzuki, N., Nonaka, Y., Yamashita, S., Miyashita, O., Ito, A., Ogasawara, S., Tama, F., Murata, T. & Uchihashi, T. Visualizing the Functional Dynamics of P-Glycoprotein and Its Modulation by Elacridar via High-Speed Atomic Force Microscopy. *Int. J. Mol. Sci.* 27, 356 (2025).
3. Shimotohno, A., Matsubayashi, Y., Du, Y., Senthilvadivel, V., Suzuki, T., Kato, H., Keshewani, M., Kono, M., Mishiro-Sato, E., Kano, K., Kojima, M., Takebayashi, Y., Sakakibara, H., Soma, F., Tama, F., Hirota, T., Torii, K. U., Yamaguchi-Shinozaki, K. & Fukuda, H. Local peptide signalling induces stomatal closure under drought stress. *Nat. Commun.* 16, (2025).
4. Wang, J., Kajiwar, K., Keshewani, M., Tama, F., Ohsaki, Y., Yamaguchi, S. & Taki, M. Single-Cell Fluorescence Analysis of Lipid Droplet Compositional Dynamics during Triacylglycerol Catabolism. *J. Am. Chem. Soc.* 147, 41514–41523 (2025).
5. Amyot, R., Miyashita, O., Wu, X., Takeda, K., Koder, N., Konno, H., Tama, F. & Flechsig, H. Flexible Fitting to Infer Atomistic-Precision Models of Large-Amplitude Conformational Dynamics in Biomolecules from High-Speed Atomic Force Microscopy Imaging. *ACS Nano* 19, 34065–34079 (2025).
6. Raghavan, S. S., Shinoda, K., Nango, E., Tama, F. & Miyashita, O. Semi-automated modeling of reaction states in time-resolved serial femtosecond crystallography using molecular dynamics sampled conformations. *Struct. Dyn.* 12, 054701 (2025).
7. Ng, K. W., Yildiz, O., Peterka, T., Tama, F., Miyashita, O., Schuman, C. & Taufer, M. Energy-Efficient Neural Network Training for Scientific Datasets with Advanced Similarity Analytics and Orchestration. *Int. Conf. Comput. Sci.* 298–312 (2025).

Oral Presentations (Invited)

1. Tama, F. Integrative modeling approaches to characterize dynamics of biomolecules. Protein Science and Engineering in the New Era Meeting, Academia Sinica (April 2025).
2. Tama, F. Bridging Cryo-EM Data and Atomic Models: Exploring Biomolecular Dynamics with MD Simulations and High-Performance Computing. PACS 2025 (June 2025).
3. Tama, F. Exploring continuous conformational variability via Cryo-EM single particle imaging and MD simulations. Annual Meeting of the Biophysical Society of Japan (September 2025).
4. Miyashita, O. Unveiling Protein Dynamics through Data Integration Simulations. 63rd Annual Meeting of the Biophysical Society of Japan (September 2025).
5. Tama, F. Integrative modeling approaches to characterize dynamics of biomolecules. Annual Meeting of the Japanese Biochemical Society (November 2025).
6. Tama, F. Conformational variability from single particle imaging. Workshop on "Program for Promoting Researches on the Supercomputer Fugaku" (November 2025).
7. Tama, F. Structure and Dynamics of Biomolecules via Integrative Modeling Approaches. Generative Design to Unlock the Potential of Protein Function Area Meeting (December 2025).
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