

ADNAN SLJOKA

NATIONALITY: Canadian

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Research interests: Computational Biology (particularly related to structural biology, protein dynamics, allostery, antibodies, GPCRs, protein structure validation), algorithm development, mathematical rigidity theory, biophysics methods, artificial intelligence and machine learning.

Research aims: To achieve scientific breakthroughs and develop innovative technologies using interdisciplinary research in applied mathematics, computational biology and artificial intelligence in order to understand the molecular mechanisms of protein function with applications to drug discovery.

WORK EXPERIENCE:

• **Research Scientist (RIKEN), Group Leader (Japan Science and technology CREST)**

(2019-present)

RIKEN, Tokyo, Japan

-carrying out multiyear funded research projects with co-supervision of postdoc and group members

• **Visiting Professor (2019-2020)**

University of Toronto, Toronto, Canada

Department of Chemical and Physical Sciences

• **Visiting Professor (2020)**

University of Hyogo, Kobe, Japan

• **Assistant Professor (2016-2019)**

Kwansei Gakuin University, Osaka, Japan

Department of Informatics, School of Science and Technology

CREST, Japan Science and Technology Agency, Japan

• **Postdoctoral Research Fellow (2015 - 2016)**

Kyoto University, Kyoto, Japan

Kwansei Gakuin University, Osaka, Japan

CREST, Japan Science and Technology Agency, Japan

<http://www.alg.cei.uec.ac.jp/itohiro/crest/eng/algorithm.html>

• **Postdoctoral Fellow (2012 – 2014)**

Department of Psychology and Neuroscience , University of Colorado Boulder (Denver, Colorado) and

Department of Physics, Ryerson University (Toronto, Canada)

• **Teaching and Research Assistant (2004 – 2012)**

Department of Mathematics and Statistics, York University: (Toronto)

-Instructed, held tutorial sessions and tutored students in Calculus of single and multi-variables, Linear Algebra, Discrete Mathematics, Mathematical Education and Business Mathematics.

- Conducted research on applied mathematics and its applications to biomedicine

- Part of NIH (USA) and NSERC (Canada) funded grant

EDUCATION:

- **Doctor of Philosophy (2012)**

Applied Mathematics, York University: (Toronto)

Dissertation title: Algorithms in rigidity theory with applications to protein flexibility and mechanical linkages,

Advisor: Walter Whiteley (see https://www.fields.utoronto.ca/programs/scientific/14-15/making_models/)

- **Master of Science (2006)**

Applied and Industrial Mathematics, York University: (Toronto)

Thesis title: *Counting for Rigidity, Flexibility and Extensions via the Pebble Game Algorithm*,

Supervisor: Walter Whiteley,

Awards: York University Best Thesis prize

- **Canadian Certificate in Bioinformatics (2005)**

Canadian Genetic Disease Network, University of British Columbia, University of Calgary, University of Montreal

- **Bachelor of Education (Teaching) (2004)**

University of Windsor: (Windsor)

Division: Intermediate/Senior, Teachable: Mathematics and Geography

Awards: Most Valuable Teaching Award

- **Bachelor of Science With Honours (2002)**

Applied Mathematics Specialized Honours, York University: (Toronto)

VISITING PROFESSOR / SCIENTIST:

- Department of Mathematics, University of Canterbury, New Zealand, Prof. Mike Steel (December 2019)

- Department of Chemical and Physical Sciences, University of Toronto, Prof. Scott Prosser, Prof. Andrew Wooley, Prof. Patrick Gunning (Medicinal Chemistry) (August, 2015, November 2016, May-June, October 2017, February-March 2018, July-August 2018)

- Department of Biochemistry, Sheffield University, UK, Prof. Mike Williamson (December 2017, February 2020)

- Robotics, Johannes Kepler University, Linz, Austria, Prof. Andreas Mueller (December 2017)

- The Center for Molecular Life Sciences, University of Basel, Prof. Stefan Grzesiek, NMR Laboratory, (July-August, 2016)

- Faculty of Engineering, Tel-Aviv University, Israel, Prof. Offer Shai (January, 2015)

- Graduate School of Engineering, Kyoto University, Kyoto, Japan (July 2013, April 2014)

- Institut de Robòtica i Informàtica Industrial, Universitat Politècnica de Catalunya, Barcelona, Spain (September 2012)

Scientific Publications:

(*Indicates first or corresponding authorship)

Submitted / Under Review:

*[28] Huang S.K., Pandey A., Tran D.T., Villanueva N.L., Kitao A., Sunahara R.K., **Sljoka A.** and Prosser R.S., Delineating the conformational landscape of the adenosine A_{2A} receptor during G protein coupling, under revision, Cell, 2020.

*[27] Wang X., Mafi A., **Sljoka A.**, Tucs A. Tsuda K., Goddard III W.A. and Ye L. Conformational Insights into Signalling Mechanism of Partial Agonism in GPCRs, submitted, 2020.

Published:

*[26] Fowler N., **Sljoka A.** and Williamson MP, A method for validating the accuracy of NMR protein structures, In press, Nature Communications, 2020

*[25] Bera S., Rashid M., Medvinsky A.B., Sun GQ, Li BL, Acquisti C, **Sljoka A.** and Chakraborty A., Allosteric regulation of Glutamate dehydrogenase deamination activity, Scientific Reports, **10**, 16523, 2020.

*[24] **Sljoka A.**, Probing Allosteric Communication with Long-range rigidity transmission across protein networks, Allostery: from physical chemistry to drug discovery, Methods in Molecular Biology, invited contribution Springer Protocols, (To Appear 2020).

[23] Rashid M., Bera S., **Sljoka A.** Chakraborty A., Feedforward Control of Plant Nitrate Transporter NRT1.1Biphasic Adaptive Activity, Biophysical Journal, <https://doi.org/10.1016/j.bpj.2019.10.018>, 2020

[22] P. Mehrabi , C. Di Pietrantonio, T.H. Kim, **A. Sljoka** , K. Taverner, C. Ing, N., R. Pomès , E.F. Pai, R.S. Prosser, Substrate-Based Allosteric Regulation of a Homodimeric Enzyme, J. Am. Chem. Soc., 141,29,11540-11556, 2019.

[21] Ye L., C. Neale, **Sljoka A.**, Pichugin D., Tsuchimura N., Sunahara R., Prosser S. et al, Bidirectional Regulation of the A_{2A} Adenosine G Protein-Coupled Receptor by Physiological Cations, Nature Communication, 1 9:1372, 2018

*[20] Jeliakov J.R., **Sljoka A.**, Kuroda D., Tsuchimura N., Katoh N., Tsumoto K., Gray J.J., Repertoire Analysis of Antibody CDR-H3 Loops Suggests Affinity Maturation Does Not Typically Result in Rigidification, Frontiers in Immunology, 9, 413, 2018.

[19] Tsuchimura S. and **Sljoka A.**, Distributed Computation for Protein Structure Analysis, The 10-th International Conference on Intelligent Networking and Collaborative Systems, (INCoS-2018), Bratislava, Slovakia, Lecture Notes in Data Engineering and Communication Technologies Series, To Appear, Springer, 2018.

*[18] **Sljoka A.** and Saitoh T., Validation of NMR protein structures using rigidity theory and chemical shifts, Journal of Information Processing Information, Research Report Bioinformatics, 2018.

[17] Deng B., Zhu S., Macklin A.M., Xu j., Lento C., **Sljoka A.**, Wilson, D., Suppressing allostery in epitope mapping experiments using millisecond hydrogen / deuterium exchange mass spectrometry, MAbs, 1:10, 2017.

[16] Kim T., Mehrabi P., **Sljoka A.**, Ing C., Bezginov A., Pomes R., Prosser S. and Pai E., The Role of Dimer Asymmetry and Protomer Dynamics in Enzyme Catalysis, Science 355, 262, 2017.

Press release: http://global.kwansei.ac.jp/news/2017/news_20170208_015101.html

[15] Cheng S.W., H. Yuya, Katoh N., **Sljoka A.**, Characterizing Minimal Rigidity of Square-Grid Frameworks with Holes. Proceedings of the 10th Japanese-Hungarian Symposium on Discrete Mathematics and Its Applications, 2017.

*[14] Hahn E., **Sljoka A.** and Muller A., Applications of Constraint Graphs and Assur groups in applications of constraint graphs and Assur groups in Mechanism Analysis and Synthesis, Proceedings of the ASME 2017 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference, IDETC2017, August 6-9, 2017, Cleveland, Ohio, USA, 2017.

*[13] Higashikawa Y., Katoh N., Kobayashi Y. and **Sljoka A.**, Characterizing redundant rigidity and redundant global rigidity of body-hinge graphs, Information Processing Letters, 116 (2), 175-178, 2016.

[12] Zhu S., Shala A., Bezginov A., **Sljoka A.**, Audette G. and Wilson D., Hyperphosphorylation of Intrinsically Disordered Tau Protein Induces an Amyloidogenic Shift in Its Conformational Ensemble, PLoS ONE, 10(3), 2015.

*[11] Nixon A., Schulze B., **Sljoka A.**, Whiteley W., Symmetry Adapted Assur Decompositions, Symmetry, 6(3), 516-550, 2014.

*[10] Porta J.M., Ros L, Schulze B., **Sljoka A.** and Whiteley W., On the Symmetric Molecular Conjectures, in Computational Kinematics, Vol 15 of Mechanisms and Machine Science, pp. 175-184, Springer, 2014.

[9] Schulze B., **Sljoka A.** and Whiteley W., How does symmetry impact the flexibility of proteins?, Philosophical Transactions of Royal Society A 372, 20120041, 2014.

*[8] **Sljoka A.** and Wilson D., *Probing Protein Ensemble Rigidity and predictions of Hydrogen-Deuterium exchange*, Physical Biology, **10** 056013, 2013.

[7] Shai O., **Sljoka A.** and Whiteley W., Directed Graphs, decompositions and Spatial Decompositions, Discrete Applied Mathematics, 161 3028–3047, 2013.

*[6] **Sljoka A.**, Shai O. and Whiteley W., *Checking Mobility and Decomposition of Linkages via Pebble Game Algorithm*, Proceedings of the ASME 2011 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference, IDETC/CIE 2011, August 29-31, 2011, Washington, DC, USA., 2011.

*[5] **Sljoka A.** and Bezginov A., *Predicting hinge motions and allostery using rigidity theory*, Advances in Mathematical and Computational Methods: Addressing Modern Challenges of Science, Technology, and Society, The International Conference on Applied Mathematics, Modeling and Computational Science, Volume 1368, pp. 167- 170, Waterloo, Canada, 2011.

[4] Schulze B., **Sljoka A.** and Whiteley W., Protein flexibility of dimers: Do symmetric motions play role in allosteric interactions, *Advances in Mathematical and Computational Methods: Addressing Modern Challenges of Science, Technology, and Society*, The International Conference on Applied Mathematics, Modeling and Computational Science, Volume 1368, pp. 135-138, Waterloo, Canada, 2011.

*[3] **Sljoka A.**, Counting for Rigidity, *Flexibility and Extensions via the Pebble Game Algorithm – Hinge Predictions and other Biological Applications* (2nd prize), Third Canadian Student Conference on Biomedical Computing, 2008.

Thesis:

[2] **Sljoka A.**, Algorithms in rigidity theory with applications to protein flexibility and mechanical linkages, PhD dissertation, York University, Toronto, 2012.

[1] **Sljoka A.**, *Counting for Rigidity, Flexibility and Extensions via the Pebble Game Algorithm*, Master's Thesis, York University, Toronto, 2006. This thesis won Best Thesis Prize.

SELECTION OF INVITED TALKS AND SEMINARS:

- Sljoka A., Rigidity of graphs for structural protein validation and functional design, IABD, Kyoto University 2019.
- Sljoka A., Lifting the curtain: probing biological secrets at molecular level with rigidity theory and algorithms, AMNS, Pokhara, 2019.
- **Keynote talk**, Rigidity theory and its applications to protein function analysis, Workshop of CREST Big Data Applications, Shonan-Village, Japan, January 16-17, 2019.
- Rigidity theory and protein function design, Central University of Rajasthan, India, November 29, 2018.
- High throughput analysis of allostery through propagation of rigidity, 3DSIG: Structural Bioinformatics and Computational Biophysics, 26th Conference on Intelligent Systems for Molecular Biology, International Society of Computational Biology, July 10, 2018, Chicago.
- Allosteric transmission across GPCR networks (poster), GPCR Structure and Function: Taking GPCR Drug Development and Discovery to the Next Level, Santa Fe, February 16-20, 2018.
- Probing allosteric communication with long-range rigidity propagation across protein networks, 100th Canadian Chemistry Conference, Toronto, Canada, May 30, 2017.
- Allosteric mechanism with propagation and experimental validations, Frontiers of NMR Life Sciences, Keystone, Colorado, March 15, 2017.
- Exploring protein flexibility and allosteric signalling mechanism with rigidity theory, 3rd Asia-Pacific World Congress on Computing Science 2016 (APWC on CSE 2016), Fiji, IEEE, Dec 5, 2016.
- Understanding protein motions and allostery with rigidity theory, McMaster University, Hamilton, Canada, Nov 22, 2016
- Recent topics in rigidity theory with applications to protein function, Graduate School of Faculty of Science, Kyoto University, November 2, 2016.

- Probing the mechanism of allosteric signal transduction in proteins with fast algorithms from rigidity theory, International Workshop on Innovative Algorithms for Big Data, Osaka, October 29, 2016.
- Probing Allosteric Communication via Transmissions of Rigidity, International Conference on Magnetic Resonance in Biological Systems (ICMRBS), Kyoto, Japan, Aug 21-26, 2016
- Topics in rigidity theory with applications to protein flexibility and allostery, University of Basel, July 26, 2016
- Detecting protein flexibility and its functions via rigidity theory, International Conference on Applications of Mathematics to Nonlinear Sciences (AMNS-2016), Kathmandu, Nepal, May 28, 2016.
- GPCR allostery using rigidity theory, G Protein-Coupled Receptors: Structure, Signaling and Drug Discovery Keystone, Colorado, Feb 21-25, 2016 (poster).
- Applications of rigidity theory to predicting protein flexibility and allosteric interactions, The Hospital for Sick Children, Toronto, March 17, 2016.
- Towards a general mechanism of allosteric communication, CREST meeting on Big Data Algorithms, Tokyo, Japan, Dec, 19, 2015.
- Probing GPCR allostery communication via transmissions of rigidity, GPCR Workshop, Hawaii, December 1-5, 2015 (poster)
- Probing rigidity and flexibility of proteins via rigidity theory, University of Toronto, July 27, 2015.
- Body-hinge Assur graphs: Inductive Construction Techniques, Advances in Combinatorial and Geometric Rigidity Theory, Banff International Research Station (BIRS), Banff, Canada, July 12, 2015.
- Allostery with rigidity theory – insights into GPCRs, CREST meeting on Big Data Algorithms, Sapporo, Japan, July, 13, 2015.
- Counting for rigidity and flexibility - applications to protein flexibility, CREST meeting on Big Data Algorithms, Ikaho, Japan, March, 20, 2015.
- Rigidity Theory and applications to protein flexibility, Japan Advanced Institute of Technology, Nomi, Japan, March, 16, 2015
- Rigidity-based allostery in GPCRs, The 28th Annual Symposium of The Protein Society, San Diego, California, July 27-31, 2014.
- A new rigidity-based model for allosteric communication in G-Protein coupled receptors, G Protein-Coupled Receptors: Structural Dynamics and Functional Implications, Snowbird, Utah, March 30th – April 4th, 2014.
- Algorithms in rigidity theory – allostery and hinge detections, Department of Biophysics, Graduate School of Science, Kyoto University, Kyoto, Japan, July 25, 2013.

- Counting for rigidity and flexibility - algorithms and applications to protein flexibility and linkage decompositions, Seminar at Institut de Robòtica i Informàtica Industrial, Barcelona, Spain, (Sept 21, 2012).
- Rigidity-based Allosteric communication (poster), Allosteric Regulation of Cell Signalling, Spanish National Cancer Research Centre, Madrid, Spain, (September 17-19, 2012).
- Predicting Rigidity and Flexibility of proteins using rigidity theory, Recomb 2011, 15th Annual International Conference on Research in Computational Molecular Biology, Vancouver, BC, (March 28, 29, 2011).
- Decomposition of Mechanisms: Assur Graphs and Algorithms, Geometry day at York, York University, Toronto, Canada, (January, 26, 2011).
- Predicting flexibility and motions of proteins using rigidity theory, MITACS / CORS 2010 Annual Conference, Edmonton, Canada, (May 25, 2010)
- Pebble Game Algorithm, Hinge predictions and allostery, Molecular Simulations: Algorithms, Analysis, and Applications, Institute of Mathematics and its Applications (IMA), University of Minnesota, Minneapolis, MN, USA (May 18, 2009)
- Pebble Game Extensions: Relevant Regions, Hinge Motions and Allostery. Recent Progress in Rigidity Theory, Banff International Research Station (BIRS), Banff, Canada (July 11, 2008)
- Third Canadian Student Conference on Biomedical Computing, Institute of Biomaterials and Biomedical Engineering, Toronto (March 13, 2008)
- Algorithms in Rigidity Theory: The Pebble Game Algorithm, York University (January 2007)

ORGANISATION OF TOP-TIER INTERNATIONAL CONFERENCES:

- Co-organizer of Conference “Workshop on Making Models: Simulating Research in Rigidity Theory and Spatial-Visual Reasoning” at Fields Institute for Research in Mathematical Sciences, Toronto, Canada, August 5-9, 2014
(see http://www.fields.utoronto.ca/programs/scientific/14-15/making_models/index.html)

FUNDING: (last 5 years)

- JST CREST (Japan) Principal Investigator, COVID-19 computational protein structure analysis and drug design (Equivalent US \$45,000) 2020-2021
- JST CREST (Japan) Principal Investigator, Protein function analysis and allostery using rigidity theory, (Equivalent US \$100,000) 2019-2020
- JST CREST (Japan) Group Co-Investigator on Multimember team, Algorithms and Applications, (Equivalent US \$3,000,000) 2015-2020
- NSERC (Canada) Co-Investigator, Technology Enhanced Biopharmaceuticals Development and Manufacturing (TEBioDev) CRD, (Equivalent US \$1,000,000) 2020-2024
- JST PRISM, Principal Investigator, NMR Validation method and Allostery Analysis, (Equivalent US \$45,000) 2018-2019
- JST AIP, Principal Investigator, NMR validation algorithms, (Equivalent US \$15,000) 2017-2018

- Biotechnology and Biological Sciences Research Council (UK), Collaborator, NMR Validation, (Equivalent US \$350,000), 2018-2021

Student and Postdoc Supervision:

- Training a Postdoctoral fellow at University of Tokyo on conformational dynamics of protein structures.
- Training a Postdoctoral fellow in Sheffield University, UK on validation of NMR structures project with Prof. Mike Williamson.
- Training of Japanese researchers belonging to CREST big data project on rigidity theory and its application to protein motions (June 2015 – ongoing)
- Mentoring of a PhD student in University of Toronto on algorithms in rigidity and applications to computational biology (June 2009 – 2016)
- Supervised a senior undergrad student's research project (York University, 2012)

Service, Community Involvement, Leadership and Other:

- Reviewer for journals Journal of Structural Biology, Nature Scientific Reports, Mechanics Based Design of Structures and Machines, An International Journal, Discrete Mathematics, ASME Mechanical Engineering and many others.
- Co-organizer of Conference “Workshop on Making Models: Simulating Research in Rigidity Theory and Spatial-Visual Reasoning” at Fields Institute for Research in Mathematical Sciences, Toronto, Canada, August 5-9, 2014
http://www.fields.utoronto.ca/programs/scientific/14-15/making_models/index.html
- Special topics in mathematics and biomedicine to enriched grade 12 classes at the Ontario Science Centre (Toronto, 2009).
- Vincent Massey Secondary School - coordinated various mathematical contests (eg. The Fryer, Galois, Hypatia, Euclid Contests) (April 2004, Windsor)
- Attended several monthly meetings at the Fields Institute for Mathematical Research with Council of Ontario Universities task force to rebuild geometry education and other revisions into the Ontario Mathematics Curriculum (Toronto, 2007 - 2009)

AWARDS, SCHOLARSHIPS AND ACHIEVEMENTS:

- Winner of PRISM Challenging research grant, Japan Science and Technology Agency, 2018-2019
- Winner of AIP Challenging research, Japan Science and Technology Agency, 2017
- CREST, Japan Science and Technology Agency Research Fellowship, 2015-2017
- Young Investigator/ Finn World Presentation Award, Annual Symposium of Protein Society, 2014, 2015
- Postdoctoral Fellowship, University of Boulder and Ryerson University, National Institute of Health (USA) 2013
- Postdoctoral Fellowship, York University, 2012
- Research Assistantship Scholarship, York University (2004 – 2011)
- Teaching Assistantship Scholarship, York University (2004 – 2011)

- Support from National Institute of Health (US) and University of Illinois at Urbana-Champaign to attend a Hands on Workshop on Computational Biophysics, Beckman Institute, University of Illinois, Urbana-Champaign, Illinois, November 1-5, 2011.
- Support from London Mathematical Society (UK) to attend London Mathematical Society Workshop: Rigidity of Frameworks and Applications, Lancaster University, Lancaster, UK, July 12-15, 2010
- Support from National Science Foundation (US) and MITACS (Canada) to attend DIMACS/MBI US-African Advanced Study Institute and workshop on Mathematical Economic Epidemiology in Kampala, Uganda, July 17 - August 5, 2009
- Performed simulation of the motion of the key mutant and nonmutant protein of Cystic Fibrosis which appeared on the film for Television of Ontario (TVO) series and Knowledge Network, *Donald Coxeter: The Man Who Saved Geometry*. <http://www.imdb.com/title/tt1541130/combined>
- Support from University of Georgia (US) to attend Summer School on Multivariate Splines and Applications, Athens, GA, May 11-22, 2009
- Poster prize, second place. Third Canadian Conference on Biomedical Computing, Toronto (May 2008)
- Best Master's Thesis Award, Faculty of Graduate Studies, York University (2006)
- Burroughs Wellcome Fund, International Competition, (To attend Genomics Workshop organized by Canadian Genetics Disease Network at University of Calgary) (May 2005)
- Canadian Institute of Health Research (CIHR) Institute of Genetics Short Term Research Visit Competition (2005) to attend the Bioinformatics, Genomics and Proteomics Workshops at University of British Columbia, University of Calgary, Université de Montréal
- MITACS Mobility Fund Award (To attend MITACS-METHEON workshop "Complex Networks in the Life Sciences" and "Minisymposium on Mathematics in the Life Sciences" in Berlin, Germany, March 29-April 04, 2007).
- Support from Pacific Institute of Mathematical Sciences (PIMS) to attend "The eighth PIMS graduate industrial math modelling camp", [University of Lethbridge](http://www.pims.ca), Lethbridge, Canada (May 7 – 11, 2005).
- Support from Pacific Institute of Mathematical Sciences (PIMS) to attend "The ninth PIMS industrial problem solving workshop", [University of Calgary](http://www.pims.ca), Calgary, Canada (May 15 – 19, 2005).
- Most Valuable Student Award, Faculty of Education, University of Windsor (2004)
- Member of Dean's and Chair's Honour Roll, York University (2000-2002)

Other activities:

- Played competitive tennis national and international level tournaments in 2000s, including Varsity Tennis, York University 1997-2002
- hiking, skiing, biking