

Dr. Didier Devaurs

XDF Research Fellow
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Education

Feb 2015 **Ph.D. in Artificial Intelligence** (with distinction), INPT, University of Toulouse, France
Dec 2006 **M.Sc. in Computer Science** (ranked first), Claude Bernard University, Lyon, France
Jan 2005 **B.Sc. in Computer Science** (ranked first), Blaise Pascal University, Clermont-Ferrand, France
May 2003 **Teacher certification in Mathematics**, IUFM of Auvergne, Clermont-Ferrand, France

Research Experience

Sep 2020 – present **XDF Research Fellow**, University of Edinburgh, MRC IGC, Edinburgh, UK.
I lead cross-disciplinary projects in quantitative biomedical research (on protein mutation interpretation, protein-protein interaction analysis, molecular docking, molecular caging, and integrative molecular modeling), with various collaborators

Dec 2018 – Aug 2020 **Postdoctoral Research Associate**, Univ. Grenoble Alpes, Inria, Grenoble, France.
Worked on achieving accurate protein-peptide binding prediction, efficient molecular caging prediction, and iterative molecular modeling using sparse experimental data

Nov 2014 – Oct 2018 **Keck Fellow & Postdoctoral Research Associate**, Rice University, Houston TX, USA.
Conceived efficient and scalable computational methods for the structural modeling and analysis of peptides, proteins, and their complexes, under Prof. Lydia Kavraki

Mar 2010 – Oct 2014 **Ph.D. candidate**, Robotics and Interactions, LAAS–CNRS, Toulouse, France.
Extended sampling-based algorithms for path planning to complex cost spaces and applied them to problems in robotics and structural biology, under Dr. Juan Cortés

Jul 2013 – Aug 2013 **Visiting Researcher**, Computer Science, George Mason University, Fairfax, USA.
Combined probabilistic search techniques from different fields to explore the energy landscape of peptides exhaustively and efficiently, under Prof. Amarda Shehu

Mar 2011 – Apr 2011 **Visiting Researcher**, Life Sciences, Barcelona Supercomputing Center, Spain.
Implemented parallel versions of sampling-based algorithms for path planning and applied them to the simulation of molecular motions, under Prof. Victor Guallar

Nov 2008 – Feb 2010 **Research Assistant**, Knowledge Services, Know-Center GmbH, Graz, Austria.
Developed modules for a technology-enhanced learning environment based on user context detection and semantic techniques, under Prof. Stefanie Lindstaedt

Oct 2007 – Sep 2008 **Research Assistant**, School of Computer Science, University of Windsor, ON, Canada.
Analyzed speciation patterns produced by an individual-based ecosystem simulation involving fuzzy cognitive maps, under Dr. Robin Gras

Oct 2006 – Sep 2007 **Research Assistant in Computer Science**, Distribcom, IRISA – Inria, Rennes, France.
Formalized the theoretical problem of performing modular diagnosis in large distributed discrete-event systems, under Dr. Eric Fabre

Additional Professional Experience

- Sep 2020 – present* **Marker**, University of Edinburgh, Biomedical Teaching Organisation, Edinburgh, UK.
Marked Masters and Honours research projects in Biomedical Sciences
- Oct 2006 – Sep 2007* **Teaching Assistant in Computer Science**, University of Rennes 1, Rennes, France.
Conducted programming tutorials and lab sessions for undergraduate students
- Apr 2005 – Aug 2005* **Software Developer**, Axemble, Charbonnières-les-Bains, France.
I devised administrative processes (marketing, finance, information system)
- Dec 2003 – Jun 2004* **Student Consultant**, Blaise Pascal University, Clermont-Ferrand, France.
I assisted students and monitored the computer center
- Sep 2002 – Aug 2003* **Mathematics Teacher**, Mortaix Secondary School, Pont-du-Château, France.
Taught a class of 24 twelve-year old students during a full academic year

Grants & Fellowships

- Feb 2023* SULSA (Scottish universities life sciences alliance) **ECR development fund** (£4K; ranked first)
- May 2022* IGC (Institute of Genetics and Cancer) **travel grant** (£2K)
- Feb 2022* SULSA (Scottish universities life sciences alliance) **ECR prize** (£3K; selectivity: 15%)
- May 2020* Cross-Disciplinary **Fellowship** (XDF) from the University of Edinburgh (£200K; selectivity: 2%)
- Mar 2018* Extreme Science and Engineering Discovery Environment (XSEDE) startup **allocation** (\$2.5K)
- Apr 2017* Computational Cancer Biology Training Program (CCBTP) postdoctoral **fellowship** (\$83K)
- May 2013* ICRA '13 student **travel grant**, from the Institute of Electrical and Electronics Engineers (€300)
- Feb 2011* HPC-Europa2 **mobility grant**, from the European Commission (€5K)
- Oct 2006* French Ministry of Education and Research's research **scholarship**
- Oct 2005* Claude Bernard University Master's degree's excellence **scholarship**

Awards & Distinctions

- Mar 2023* finalist in the **STEM for BRITAIN** poster competition, Houses of Parliament, London, UK
- Apr 2020* selection for the **MSCA MaRaThoN** @ University of Padua (grant writing workshop), Italy
- Sep 2018* 9th ACM int conf bioinformatics, computational biology & health informatics (BCB) **poster award**
- Aug 2018* 4th Annual Smalley-Curl Institute Summer Research Colloquium's **poster award**
- Apr 2018* 23rd Sealy Center for Structural Biology and Molecular Biophysics Symposium's **poster award**
- Oct 2017* 27th Annual Keck Center Research Conference's **poster award**
- May 2017* 22nd Sealy Center for Structural Biology and Molecular Biophysics Symposium's **poster award**
- Mar 2017* selection for **ComSciCon** Houston (science communication workshop), USA
- Apr 2016* 21st Sealy Center for Structural Biology and Molecular Biophysics Symposium's **poster award**
- Dec 2014* Léopold Escande **Ph.D. award**, University of Toulouse, France

Publications

Journal Publications

26. Anja Conev, Mauricio M. Rigo, **Didier Devaurs**, André F. Fonseca, Hussain Kalavadwala, Martiela V. de Freitas, Cecilia Clementi, Geancarlo Zanatta, Dinler A. Antunes, Lydia E. Kavraki. *EnGens: a computational framework for generation and analysis of representative protein conformational ensembles*. Submitted to Briefings in Bioinformatics, 2023
25. Anja Conev, **Didier Devaurs**, Mauricio M. Rigo, Dinler A. Antunes, Lydia E. Kavraki. *3pHLA-score improves structure-based peptide-HLA binding affinity prediction*. Scientific Reports 12(1): 10749, 2022, doi: 10.1038/s41598-022-14526-x
24. **Didier Devaurs**, Dinler A. Antunes, Antoni J. Borysik. *Computational modeling of molecular structures guided by hydrogen-exchange data*. Journal of the American Society for Mass Spectrometry 33(2):215-237, 2022, doi: 10.1021/jasms.1c00328. **Featured as cover article**
23. Sarah Hall-Swan*, **Didier Devaurs***, Mauricio M. Rigo, Dinler A. Antunes, Lydia E. Kavraki, Geancarlo Zanatta. *DINC-COVID: A webserver for ensemble docking with flexible SARS-CoV-2 proteins*. Computers in Biology and Medicine 139, 2021, doi: 10.1016/j.compbiomed.2021.104943 (* **shared first-authorship**)
22. **Didier Devaurs**, Dinler A. Antunes, Lydia E. Kavraki. *Computational analysis of complement inhibitor compstatin using molecular dynamics*. Journal of Molecular Modeling 26(9):231, 2020, doi: 10.1007/s00894-020-04472-8
21. Dinler A. Antunes, Jayvee R. Abella, Sarah Hall-Swan, **Didier Devaurs**, Anja Conev, Mark Moll, Gregory Lizée, Lydia E. Kavraki. *HLA-Arena: A customizable environment for the structural modeling and analysis of peptide-HLA complexes for cancer immunotherapy*. JCO Clinical Cancer Informatics 4: 623-636, 2020, doi: 10.1200/CCI.19.00123
20. Oleksandr Kravchenko, Anastasiia Varava, Florian T. Pokorny, **Didier Devaurs**, Lydia E. Kavraki, Danica Kragic. *A robotics-inspired screening algorithm for molecular caging prediction*. Journal of Chemical Information and Modeling 60(3):1302-1316, 2020, doi: 10.1021/acs.jcim.9b00945
19. **Didier Devaurs**, Dinler A. Antunes, Sarah Hall-Swan, Nicole Mitchell, Mark Moll, Gregory Lizée, Lydia E. Kavraki. *Using parallelized incremental meta-docking can solve the conformational sampling issue when docking large ligands to proteins*. BMC Molecular and Cell Biology 20(1):42, 2019, doi: 10.1186/s12860-019-0218-z
18. Dinler A. Antunes, Jayvee R. Abella, **Didier Devaurs**, Mauricio M. Rigo, Lydia E. Kavraki. *Structure-based methods for binding mode and binding affinity prediction for peptide-MHC complexes*. Current Topics in Medicinal Chemistry 18(26): 2239-2255, 2018, doi: 10.2174/1568026619666181224101744
17. **Didier Devaurs**, Dinler A. Antunes, Lydia E. Kavraki. *Revealing unknown protein structures using computational conformational sampling guided by experimental hydrogen-exchange data*. International Journal of Molecular Sciences 19(11): 3406, 2018, doi: 10.3390/ijms19113406
16. Dinler A. Antunes, **Didier Devaurs**, Mark Moll, Gregory Lizée, Lydia E. Kavraki. *General prediction of peptide-MHC binding modes using incremental docking: A proof of concept*. Scientific Reports 8(1):4327, 2018, doi: 10.1038/s41598-018-22173-4
15. **Didier Devaurs**, Malvina Papanastasiou, Dinler A. Antunes, Jayvee R. Abella, Mark Moll, Daniel Ricklin, John D. Lambris, Lydia E. Kavraki. *Native state of complement protein C3d analysed via hydrogen exchange and conformational sampling*. International Journal of Computational Biology and Drug Design 11(1/2):90-113, 2018, doi: 10.1504/IJCBDD.2018.10011903

14. Dinler A. Antunes, Mark Moll, **Didier Devaurs**, Kyle R. Jackson, Gregory Lizée, Lydia E. Kavraki. *DINC 2.0: A new protein-peptide docking webserver using an incremental approach*. Cancer Research 77(21):e55-e57, 2017, doi: 10.1158/0008-5472.CAN-17-0511
13. **Didier Devaurs**, Dinler A. Antunes, Malvina Papanastasiou, Mark Moll, Daniel Ricklin, John D. Lambris, Lydia E. Kavraki. *Coarse-grained conformational sampling of protein structure improves the fit to experimental hydrogen-exchange data*. Frontiers in Molecular Biosciences 4(13), 2017, doi: 10.3389/fmolb.2017.00013
12. Anastasia Novinskaya*, **Didier Devaurs***, Mark Moll, Lydia E. Kavraki. *Defining low-dimensional projections to guide protein conformational sampling*. Journal of Computational Biology 24(1):79-89, 2017, doi: 10.1089/cmb.2016.0144 (* **shared first-authorship**)
11. **Didier Devaurs**, Thierry Siméon, Juan Cortés. *Optimal path planning in complex cost spaces with sampling-based algorithms*. IEEE Transactions on Automation Science and Engineering 13(2):415-424, 2016, doi: 10.1109/TASE.2015.2487881
10. Dinler A. Antunes*, **Didier Devaurs***, Lydia E. Kavraki. *Understanding the challenges of protein flexibility in drug design*. Expert Opinion on Drug Discovery 10(12):1301-1313, 2015, doi: 10.1517/17460441.2015.1094458 (* **shared first-authorship**)
09. **Didier Devaurs**, Kevin Molloy, Marc Vaisset, Amarda Shehu, Thierry Siméon, Juan Cortés. *Characterizing energy landscapes of peptides using a combination of stochastic algorithms*. IEEE Transactions on NanoBioscience 14(5):545-552, 2015, doi: 10.1109/TNB.2015.2424597
08. **Didier Devaurs**, Léa Bouard, Marc Vaisset, Christophe Zanon, Ibrahim Al-Bluwi, Romain Iehl, Thierry Siméon, Juan Cortés. *MoMA-LigPath: A web server to simulate protein-ligand unbinding*. Nucleic Acids Research 41(W1):w297-w302, 2013, doi: 10.1093/nar/gkt380
07. **Didier Devaurs**, Thierry Siméon, Juan Cortés. *Parallelizing RRT on large-scale distributed-memory architectures*. IEEE Transactions on Robotics 29(2):571-579, 2013, doi: 10.1109/TRO.2013.2239571
06. **Didier Devaurs**, Andreas S. Rath, Stefanie N. Lindstaedt. *Exploiting the user interaction context for automatic task detection*. Applied Artificial Intelligence 26(1-2):58-80, 2012, doi: 10.1080/08839514.2012.629522
05. Johannes Moskaliuk, Andreas S. Rath, **Didier Devaurs**, Nicolas Weber, Stefanie N. Lindstaedt, Joachim Kimmerle, Ulrike Cress. *Automatic detection of accommodation steps as an indicator of knowledge maturing*. Interacting with Computers 23(3):247-255, 2011, doi: 10.1016/j.intcom.2011.03.006
04. Andreas S. Rath, **Didier Devaurs**, Stefanie N. Lindstaedt. *An ontology-based approach for detecting knowledge intensive tasks*. Journal of Digital Information Management 9(1):9-18, 2011
03. **Didier Devaurs**, Robin Gras. *Species abundance patterns in an ecosystem simulation studied through Fisher's logseries*. Simulation Modelling Practice & Theory 18(1):100-123, 2010, doi: 10.1016/j.simpat.2009.09.012
02. Michael Granitzer, Andreas S. Rath, Mark Kröll, Christin Seifert, Doris Ipsmiller, **Didier Devaurs**, Nicolas Weber, Stefanie N. Lindstaedt. *Machine learning based work task classification*. Journal of Digital Information Management 7(5):306-313, 2009
01. Robin Gras, **Didier Devaurs**, Adrianna Wozniak, Adam Aspinall. *An individual-based evolving predator-prey ecosystem simulation using a fuzzy cognitive map as the behavior model*. Artificial Life 15(4):423-463, 2009, doi: 10.1162/artl.2009.Gras.012

Conference Proceedings

8. **Didier Devaurs**, Amarda Shehu, Thierry Siméon, Juan Cortés. *Sampling-based methods for a full characterization of energy landscapes of small peptides*. IEEE International Conference on Bioinformatics and Biomedicine (BIBM); 11/2014
7. **Didier Devaurs**, Thierry Siméon, Juan Cortés. *A multi-tree extension of the Transition-based RRT: Application to ordering-and-pathfinding problems in continuous cost spaces*. IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS); 09/2014
6. Montserrat Manubens, **Didier Devaurs**, Lluís Ros, Juan Cortés. *Motion planning for 6-D manipulation with aerial towed-cable systems*. Robotics: Science and Systems (RSS); 06/2013
5. **Didier Devaurs**, Thierry Siméon, Juan Cortés. *Enhancing the Transition-based RRT to deal with complex cost spaces*. IEEE International Conference on Robotics and Automation (ICRA); 05/2013
4. **Didier Devaurs**, Thierry Siméon, Juan Cortés. *Parallelizing RRT on distributed-memory architectures*. IEEE International Conference on Robotics and Automation (ICRA); 05/2011
3. Andreas S. Rath, **Didier Devaurs**, Stefanie N. Lindstaedt. *Studying the factors influencing automatic user task detection on the computer desktop*. EC-TEL; 09/2010. **Finalist for best paper award**
2. **Didier Devaurs**, Fabien De Marchi, Mohand-Said Hacid. *Caractérisation des transitions temporisées dans les logs de conversation de services Web*. Extraction et gestion des connaissances (EGC); 01/2007
1. **Didier Devaurs**, Fabien De Marchi. *Génération de bases de transactions synthétiques : vers la prise en compte des bordures*. Bases de Données Avancées (BDA); 01/2005

Workshop / Symposium Proceedings

5. Anastasia Novinskaya, **Didier Devaurs**, Mark Moll, Lydia E. Kavraki. *Improving protein conformational sampling by using guiding projections*. Computational Structural Bioinformatics (at BIBM); 10/2015
4. **Didier Devaurs**, Marc Vaisset, Thierry Siméon, Juan Cortés. *A multi-tree approach to compute transition paths on energy landscapes*. Artificial Intelligence and Robotics Methods in Computational Biology; 07/2013
3. Montserrat Manubens, **Didier Devaurs**, Lluís Ros, Juan Cortés. *A motion planning approach to 6-D manipulation with aerial towed-cable systems*. International Micro Air Vehicle Conference and Flight Competition (IMAV); 09/2013
2. Andreas Rath, **Didier Devaurs**, Stefanie Lindstaedt. *Detecting real user tasks by training on laboratory contextual attention metadata*. Exploitation of Usage and Attention Metadata (at Informatik); 09/2009
1. Andreas Rath, **Didier Devaurs**, Stefanie Lindstaedt. *UICO: An ontology-based user interaction context model for automatic task detection on the computer desktop*. Context Information & Ontology (at ESWC); 06/2009

Poster / Demonstration Proceedings

5. Dinler Antunes, Jayvee Abella, Sarah Hall-Swan, **Didier Devaurs**, Anja Conev, Mark Moll, Gregory Lizée, Lydia Kavraki. *Virtual screening of peptide-targets for cancer immunotherapy using HLA-Arena*. International Symposium on Mathematical and Computational Oncology (ISMCO); 10/2020
4. Montserrat Manubens, **Didier Devaurs**, Lluís Ros, Juan Cortés. *Aerial 6-dimensional quasi-static manipulation on the FlyCrane towed-cable system*. RSS Workshop on Aerial Mobile Manipulation; 06/2013
3. Andreas S. Rath, **Didier Devaurs**, Stefanie N. Lindstaedt. *Contextualized knowledge services for personalized learner support*. European Conference on Technology Enhanced Learning (EC-TEL); 09/2009

2. Andreas S. Rath, **Didier Devaurs**, Stefanie N. Lindstaedt. *KnowSe: Fostering user interaction context awareness*. European Conference on Computer-Supported Cooperative Work (ECSCW); 09/2009
1. **Didier Devaurs**, Kreshnik Musaraj, Fabien De Marchi, Mohand-Said Hacid. *Timed transition discovery from web service conversation logs*. CAiSE Forum; 06/2008

Book Chapter

Didier Devaurs, Thierry Siméon, Juan Cortés. *Efficient sampling-based approaches to optimal path planning in complex cost spaces*. Algorithmic Foundations of Robotics XI (selected contributions from WAFR '14), 2015: pages 143-159; Springer, doi: 10.1007/978-3-319-16595-0_9

Ph.D. Thesis

Extensions of Sampling-based Approaches to Path Planning in Complex Cost Spaces: Applications to Robotics and Structural Biology. INPT, **University of Toulouse**, 10/2014

Talks and Presentations

Invited Talks

13. *A tale of two strategies to efficiently explore the conformational space of molecular systems*. School of Health and Life Sciences seminar, **University of the West of Scotland**, Glasgow, UK, 03/2023
12. *A tale of two strategies to efficiently explore the conformational space of molecular systems*. Glasgow cancer seminar series, **Beatson Institute for Cancer Research**, Glasgow, UK, 03/2023
11. *A tale of two strategies to efficiently explore the conformational space of molecular systems*. Institute of Medical Sciences seminar, **University of Aberdeen**, UK, 11/2022
10. *A tale of two strategies to efficiently explore the conformational space of molecular systems*. Biomedical Sciences Research Complex seminar, **University of St Andrews**, UK, 10/2022
9. *A tale of two strategies to efficiently explore the conformational space of molecular systems*. Gene Regulation and Expression seminar, School of Life Sciences, **University of Dundee**, UK, 10/2022
8. *Lessons learned from modelling data, robots and molecules*. Career development talk for the UKRI Centre for Doctoral Training in Biomedical AI, **University of Edinburgh**, UK, 11/2021
7. *Studying protein structure using HDX-MS and multi-resolution conformational sampling*. Online seminar of the **International Society for HDX-MS**, 09/2021
6. *Lessons learned from modelling data, robots and molecules*. Kavraki Group seminar (online), **Rice University**, Houston (TX), USA, 04/2020
5. *Modeling intrinsically disordered regions in proteins*. Computational Structural Biology Group seminar, **University of Basel**, Switzerland, 01/2020
4. *Efficient strategies to explore the conformational space of proteins and molecular complexes*. ABS Seminar, **Inria** Sophia Antipolis - Méditerranée, France, 11/2019
3. *Efficient strategies to explore the conformational space of proteins and molecular complexes*. CAPSID Seminar, **Loria** (Inria, CNRS, University of Lorraine), Nancy, France, 09/2019

2. *Efficient strategies to explore the conformational space of proteins and molecular complexes*. Functionality and Protein Engineering Unit seminar, **University of Nantes**, France, 09/2019
1. *Efficiently exploring the conformational space of proteins and molecular complexes*. GRAND Seminar, **George Mason University**, Fairfax (VA), USA, 08/2018

Oral Presentations

7. *Statistical modelling of longitudinal trajectories of white blood cells*. Generation Scotland team meeting; Edinburgh, UK; 04/2021
6. *Studying protein structure through hydrogen exchange and coarse-grained conformational sampling*. GT MASIM; Paris, France; 11/2019
5. *General prediction of peptide-MHC binding modes using incremental docking: A proof of concept*. ACM Int. Conf. Bioinformatics, Computational Biology & Health Informatics (BCB); Washington DC, USA; 09/2018
4. *Studying protein structure through hydrogen exchange and conformational sampling*. Smalley-Curl Institute Summer Research Colloquium (SCI SRC); Houston TX, USA; 08/2017
3. *Native state of complement protein C3d analyzed via hydrogen exchange and conformational sampling*. International Conference on Intelligent Biology and Medicine (ICIBM); Houston TX, USA; 12/2016
2. *Efficient sampling-based approaches to optimal path planning in complex cost spaces*. Workshop on the Algorithmic Foundations of Robotics (WAFR); Istanbul, Turkey; 09/2014
1. *MoMA-LigPath: A web server to simulate protein-ligand unbinding*. French Conference on Biology, Computer Science and Mathematics (JOBIM); Toulouse, France; 07/2013

Poster Presentations

14. *Making deep mutational scanning actionable to interpret protein variant effects*. STEM for BRITAIN poster exhibition; Biological and Biomedical Sciences section; London, UK; 03/2023.
13. *Computational modeling of molecular structures guided by experimental HDX-MS data*. International Conference on HDX-MS; London, UK; 04/2022. **Selected for poster flash talk**
12. *Guiding protein conformational sampling with experimental hydrogen exchange data to uncover unknown structures*. GT MASIM; Paris, France; 11/2019
11. *Guiding protein conformational sampling with experimental hydrogen exchange data to uncover unknown structures*. ACM BCB; Washington DC, USA; 09/2018. **Poster award**
10. *Guiding protein conformational sampling with hydrogen exchange data to uncover unknown structures*. Smalley-Curl institute summer research colloquium SCI-SRC; Houston TX, USA; 08/2018. **Poster award**
09. *Predicting binding modes of peptide-HLA complexes with molecular docking*. Annual Sealy Center for Structural Biology & Molecular Biophysics Symposium; Galveston TX, USA; 04/2018. **Poster award**
08. *Predicting binding modes of peptide-HLA complexes with molecular docking*. Innovations in Cancer Prevention and Research Conference; Austin TX, USA; 11/2017
07. *Predicting binding modes of peptide-HLA complexes with molecular docking*. Annual Keck Center Research Conference; Houston TX, USA; 10/2017. **Poster award**
06. *Studying protein structure through hydrogen exchange and conformational sampling*. MD Anderson Cancer Center's Annual Postdoctoral Science Symposium; Houston TX, USA; 09/2017

05. *Studying protein structure through hydrogen exchange and conformational sampling*. Annual Sealy Center for Structural Biology & Molecular Biophysics Symposium; Galveston TX, USA; 05/2017. **Poster award**
04. *Guiding protein conformational sampling with experimental HDX-MS data*. Annual Sealy Center for Structural Biology & Molecular Biophysics Symposium; Galveston TX, USA; 04/2016. **Poster award**
03. *Exploring protein conformational space using robotic path planning techniques*. Annual Keck Center Research Conference; Houston TX, USA; 10/2015
02. *Biomedical computing: Generating, analyzing and visualizing complex high-dimensional data*. Rice University Data Science Meetup; Houston TX, USA; 09/2015
01. *Exploring protein conformational space using robotic path planning techniques*. Annual Sealy Center for Structural Biology & Molecular Biophysics Symposium; Galveston TX, USA; 05/2015

Academic Advising

Primary Advising

University of Edinburgh

- Xinyu Liu, M.Sc.R in biomedical sciences (2023)
- Zihan Kong, M.Sc. in bioinformatics (2023)
- Tianyu Zhao, M.Sc. in bioinformatics (2023)
- Nicole Li, pharmacology Honours (2023)
- Natalie Cruz, biomedical sciences Honours (2023)
- Erika Lapienyte, biomedical sciences Honours (2023)
- Mengze Zhang, M.Sc.R in biomedical sciences (2022)
- Jie Mei, M.Sc. in drug discovery and translational biology (2022)
- Tiefeng Song, M.Sc. in drug discovery and translational biology (2022)

Rice University

- Anja Conev, undergraduate student (2018)
- Nicole Mitchell, undergraduate student (2018)
- Elizabeth Palmi, undergraduate student (2018)
- Stephen Price, undergraduate student (2018)
- Sarah Hall-Swan, undergraduate student (2017)
- Angela Hoch, undergraduate student (2017)
- Yovahn Hoole, undergraduate student (2017)

Graz University of Technology

- Stefanie Wechtitsch, graduate student (2009)

University of Windsor

- Mike Lee, undergraduate student (2008)

Secondary Advising

Rice University

- Anja Conev, Ph.D. student (2019 - 2022)
- Sarah Hall-Swan, Ph.D. student (2018 - 2021)
- Eleni Litsa, Ph.D. student (2018)
- Sarah Kim, Ph.D. student (2016 - 2018)
- Jayvee Abella, Ph.D. student (2015 - 2017)
- Stephen Butler, graduate student (2016)
- Anastasia Novinskaya, graduate student (2015 - 2016)

- Konstantinos Varvarezos, undergraduate student (2015)

M.Sc. Theses Fully Supervised

University of
Edinburgh

- Jie Mei. *Integrative Rosetta Molecular Modelling Guided by Experimental Hydrogen-Exchange Data*. 2022
- Tiefeng Song. *HDX-Rosetta: A Computational Tool Using Experimental HDX Data Directly to Obtain Conformation-Specific Protein Models*. 2022
- Mengze Zhang. *HDX-Rosetta: Conformational Simulation of Protein Structure Guided by Hydrogen-Exchange Data*. 2022

M.Sc. Theses Partially Supervised

Rice University

- Jayvee Abella. *Scaling up Robotics-Inspired Conformational Sampling Algorithms*. 2016
- Ryan Lear. *Supervised Classification of Motion Graphs for Swarm Robotics*. 2016
- Anastasia Novinskaya. *Improving Protein Conformational Sampling by Using Guiding Projections*. 2016

Editorial and Reviewing Activities

Editorial Board Member of Journals

- Biochemistry and Biophysics Reports: 2021 – 2023
- Biophysical Reviews: since 2018
- BMC Bioinformatics: since 2022
- Current Proteomics: 2019 – 2021
- Frontiers in Molecular Biosciences (Biological Modeling and Simulation): since 2022

Guest Editor for Journal Special Issues

- Antibiotics: 2021 (Structures and functions of antimicrobial peptides)

Topical Advisory Panel Member of Journals

- Antibiotics: since 2022
- Biomolecules: since 2022
- Pharmaceuticals: since 2022
- Vaccines: since 2022

Review Board Member of Journals

- Antibiotics: since 2020
- Frontiers in Bioengineering and Biotechnology (Nanobiotechnology): since 2021
- Frontiers in Bioinformatics (Drug Discovery in Bioinformatics): since 2021
- Frontiers in Drug Discovery (In silico Methods and AI for Drug Discovery): since 2022
- Frontiers in Molecular Biosciences (Nanobiotechnology): since 2021

Program Committee Member for Conferences

- ACM Int. Conference on Bioinformatics, Computational Biology, and Health Informatics: BCB '17
- European Conference on Computational Biology: ECCB '21
- Intelligent Systems for Molecular Biology: ISMB '21
- International Conference on Bioinformatics and Computational Biology: BICOB '19
- International Conference on Digital Information Management: ICDIM '18

Organizing Committee Member for Conferences

- International Conference on Knowledge Management and Knowledge Technologies: I-KNOW '09

Reviewer of Conference Articles

- IEEE Conference on Decision and Control: CDC '07
- IEEE International Conference on Robotics and Automation: ICRA '14, ICRA '15, ICRA '17
- IEEE/RSJ International Conference on Intelligent Robots and Systems: IROS '14
- International Conference on Methods and Models in Automation and Robotics: MMAR '16
- Robotics: Science and Systems: RSS '16
- Workshop on Algorithmic Foundations of Robotics: WAFR '14

Reviewer of Book Proposal

- Elsevier - Medicinal, Organic and Inorganic Chemistry: 2022

Reviewer of Research Proposal

- Czech Science Foundation: 2016

Reviewer of Journal Articles

- 2023 Cells
- 2022 Acta Crystallographica Section F, Antibiotics, BMC Bioinformatics, Computation, Computational Biology and Chemistry, Computers in Biology and Medicine, Expert Systems with Applications, Frontiers in Bioinformatics, Journal of Computer-Aided Molecular Design, Pharmaceuticals
- 2021 Biomolecules, COVID, Frontiers in Molecular Biosciences, Intelligence-Based Medicine, International Journal of Molecular Sciences, Journal of Chemical Theory and Computation, Scientia Pharmaceutica, Scientific Reports, Vaccines
- 2020 Antibodies, Biology, Genes, Informatics in Medicine Unlocked, JCO Clinical Cancer Informatics, Journal of Chemical Information and Modeling, Journal of Computational Biophysics and Chemistry, Journal of Theoretical and Computational Chemistry, Molecules, RSC Advances
- 2019 Applied Sciences, Autonomous Robots, Bioinformatics, IEEE Transactions on Automation Science and Engineering, Journal of Bioinformatics and Computational Biology, Sensors
- 2018 Communications in Information and Systems, IEEE Robotics and Automation Letters, International Journal of Computational Biology and Drug Design, Journal of Digital Information Management
- 2016 ACM Computing Surveys, IEEE Robotics and Automation Letters, International Journal of Robotics Research, Journal of Computational Biology
- 2015 Journal of Computational Chemistry

Scientific Collaborations

<i>since 2022</i>	Dr. Areta Czerwinska, International Institute of Molecular and Cell Biology, Warsaw, Poland
<i>since 2021</i>	Dr. Shay Cohen, School of Informatics, University of Edinburgh, UK
<i>since 2021</i>	Dr. Grzegorz Kudla, Institute of Genetics and Cancer, University of Edinburgh, UK
<i>since 2021</i>	Dr. Joseph Marsh, Institute of Genetics and Cancer, University of Edinburgh, UK
<i>since 2021</i>	Dr. Graciela Muniz-Terrera, Centre for Clinical Brain Sciences, University of Edinburgh, UK
<i>since 2021</i>	Dr. Riccardo Marioni, Institute of Genetics and Cancer, University of Edinburgh, UK
<i>since 2021</i>	Dr. Antoni Borysik, Department of Chemistry, King's College London, UK
<i>since 2020</i>	Prof. J. Douglas Armstrong, School of Informatics, University of Edinburgh, UK
<i>since 2020</i>	Dr. Adam Byron, Institute of Genetics and Cancer, University of Edinburgh, UK
<i>since 2020</i>	Dr. Geancarlo Zanatta, Department of Physics, Federal University of Ceará, Fortaleza-CE, Brazil
<i>since 2019</i>	Dr. Alexander Kravchenko, KTH Royal Institute of Technology, Stockholm, Sweden
<i>since 2018</i>	Dr. Anastasiia Varava, KTH Royal Institute of Technology, Stockholm, Sweden
<i>since 2018</i>	Dr. Mauricio Rigo, Department of Computer Science, Rice University, Houston TX, USA
<i>since 2014</i>	Dr. Dinler Antunes, Department of Biology and Biochemistry, University of Houston, TX, USA
<i>2021 – 2022</i>	Dr. Diego Oyarzún, School of Informatics, University of Edinburgh, UK
<i>2019 – 2021</i>	Dr. Emanuele Paci, School of Molecular and Cellular Biology, University of Leeds, UK
<i>2018 – 2020</i>	Dr. Sergei Grudinin, University of Grenoble Alpes, Grenoble, France
<i>2017 – 2020</i>	Prof. Gregory Lizée, The University of Texas MD Anderson Cancer Center, Houston TX, USA
<i>2014 – 2020</i>	Dr. Mark Moll, Department of Computer Science, Rice University, Houston TX, USA
<i>2017 – 2018</i>	Dr. Nidhi Sahni, The University of Texas MD Anderson Cancer Center, Houston TX, USA
<i>2014 – 2018</i>	Dr. Malvina Papanastasiou, School of Medicine, University of Pennsylvania, Philadelphia, USA
<i>2014 – 2018</i>	Dr. Daniel Ricklin, School of Medicine, University of Pennsylvania, Philadelphia PA, USA
<i>2014 – 2018</i>	Prof. John Lambris, School of Medicine, University of Pennsylvania, Philadelphia PA, USA
<i>2010 – 2016</i>	Dr. Thierry Siméon, Robotics and Interactions, LAAS-CNRS, Toulouse, France
<i>2012 – 2013</i>	Dr. Montserrat Manubens, IRI, Polytechnic University of Catalonia, Barcelona, Spain

Contributed Software

<i>DINC-COVID</i>	Ensemble docking to SARS-CoV-2 proteins – dinc-covid.kavrakilab.org
<i>DINC</i>	Docking INCrementally – dinc.kavrakilab.org
<i>HLA-Arena</i>	Structural modeling/analysis of peptide-HLA complexes – github.com/KavraKiLab/hla-arena
<i>PEPSI-SAXS</i>	Polynomial Expansions of Protein Structures and Interactions, applied to Small-Angle X-ray Scattering – team.inria.fr/nano-d/software/pepsi-saxs

SIMS Structured Intuitive Move Selector

MoMA LigPath Molecular Motion Algorithms – moma.laas.fr

Move3D Motion planning for robots – www.openrobots.org/wiki/move3d

KnowSe User context detection as a knowledge service

EcoSim Individual-based ecosystem simulation – sites.google.com/site/ecosimgroup

Scientific Societies

2021 – 2023 International Society for HDX-MS (IS-HDXMS)

2022 American Chemical Society (ACS)

2018 – 2019 ACM special interest group on bioinformatics, computational biology & biomedical informatics

2013 - 2014 Institute of Electrical and Electronics Engineers (IEEE)

Public Engagement

Mar 2023 Poster presentation at the **STEM for BRITAIN** exhibition organized by the Parliamentary and Scientific Committee in the Houses of Parliament (in London, UK), during British science week. Category: biological and biomedical sciences. Title: *Interpreting the health impact of genetic variation via deep mutational scanning and machine learning*

Mar 2023 Represented SULSA (Scottish universities life sciences alliance) as an early career researcher at **Scotland's Life Sciences Annual Dinner and Awards** ceremony, organized by the Life Sciences Scotland Industry Leadership Group in Edinburgh, UK

Mar 2020 Research mentioned in a **press release** (by Primeur Magazine, The Medical News, Newswise, and Sciencenewsnet.in). Title: *Supercomputer helps benchmark cancer immunotherapy tool*

Mar 2017 Selected for **ComSciCon Houston** (USA), a science communication workshop

Miscellaneous

<i>Languages</i>	French (mother tongue)	English (fluent)	Spanish (advanced)
	German (intermediate)	Polish (beginner)	Hindi (beginner)

<i>Computer programming</i>	Python	R	C / C++	Java	Pascal	Ada	Mathematica	Octave
	message passing (Open MPI, Boost MPI)					multi-threading (Open MP)		
	web programming (JavaScript, ActionScript, Flex, MXML, XML, PHP, HTML)							

<i>Volunteering experience</i>	2003: creation of a mathematics workshop for a children's literature festival 2003: conception of a radio internship for English students 2002 – 2003: participation in the organization of a music festival 2000 – 2004: audio technician in a community radio station
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