Didier Devaurs
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Computer And Information Sciences
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Personal Statement

I am a lecturer in the Department of Computer and Information Sciences, at the University of Strathclyde, which I joined in June 2024. I have a diverse background in computer science, mathematics, biology, and chemistry. Before jumping into academia, I had experiences as a software developer in industry and as a mathematics teacher in secondary education. I am now avidly interested in interdisciplinary research in the fields of biomolecular artificial intelligence and structural bioinformatics. I also teach courses in bioinformatics and artificial intelligence.
I currently serve on the editorial board of three scientific journals: BMC Bioinformatics, Biomolecules, and Frontiers in Molecular Biosciences. I have published 26 articles (including 15 as first author) in international scientific journals, and 19 articles (including 9 as first author) in peer-reviewed conferences or workshops. Some of my articles have garnered a sizeable number of citations, including four articles with more than 100 citations. So far, I have attracted about £300K in research funding, via two postdoctoral fellowships and small competitive grants. I have delivered 49 invited talks, oral presentations, or poster presentations, across the world. I have supervised 7 graduate and 11 undergraduate students who had either a computer science or a biology background.
If you are a motivated student looking for a supervisor to work on a project related to one of my areas of expertise (listed below), do not hesitate to contact me.

Qualifications

Doctor of Science, Ph.D. in Artificial Intelligence, LAAS-CNRS, Université de Toulouse, Toulouse, France
Award Date: 1 Feb 2015

Master of Science, M.Sc. in Computer Science, University of Lyon
Award Date: 1 Dec 2006

Bachelor of Science, B.Sc. in Computer Science, Université Clermont Auvergne
Award Date: 1 Dec 2004

Teacher Certification in Mathematics, Université Clermont Auvergne
Award Date: 1 May 2003

Projects

Moray endowment fund
Devaurs, D. (Principal Investigator) & Czerwinska, A. (Co-investigator)
1/12/23 → 31/07/24

SULSA ECR development fund
Devaurs, D. (Principal Investigator) & Czerwinska, A. (Co-investigator)
1/02/23 → 31/01/24

XDF: Cross-Disciplinary Fellowship
Devaurs, D. (Principal Investigator)
1/09/20 → 31/05/24

XSEDE start-up allocation
Devaurs, D. (Principal Investigator)
1/03/18 → 31/10/18

Keck postdoctoral fellowship
Devaurs, D. (Principal Investigator)

1/04/17 → 31/10/18

HPC-Europa2 mobility grant
Devaurs, D. (Principal Investigator)
1/02/11 → 31/05/11

Research outputs

EnGens: a computational framework for generation and analysis of representative protein conformational ensembles
Conev, A., Rigo, M. M., Devaurs, D., Fonseca, A. F., Kalavadwala, H., de Freitas, M. V., Clementi, C., Zanatta, G., Antunes, D. A. & Kavraki, L. E., 7 Jul 2023, In: Briefings in Bioinformatics. 24, 4, 11 p., bbad242.

3pHLA-score improves structure-based peptide-HLA binding affinity prediction
Conev, A., Devaurs, D., Rigo, M. M., Antunes, D. A. & Kavraki, L. E., 24 Jun 2022, In: Scientific Reports. 12, 1, 11 p., 10749.

Computational modeling of molecular structures guided by hydrogen-exchange data
Devaurs, D., Antunes, D. A. & Borysik, A. J., 2 Feb 2022, In: Journal of the American Society for Mass Spectrometry. 33, 2 , p. 215-237 23 p.

DINC-COVID: a webserver for ensemble docking with flexible SARS-CoV-2 proteins
Hall-Swan, S., Devaurs, D., Rigo, M. M., Antunes, D. A., Kavraki, L. E. & Zanatta, G., 1 Dec 2021, In: Computers in Biology and Medicine. 139, 21 p., 104943.

DINC-COVID: Ensemble docking against flexible SARS-CoV-2 proteins
Devaurs, D. (Developer), 2021

Virtual screening of peptide-targets for cancer immunotherapy using HLA-Arena
Antunes, D. A., Abella, J. R., Hall-Swan, S., Devaurs, D., Conev, A., Moll, M., Lizée, G. & Kavraki, L. E., 1 Oct 2020, *International Symposium on Mathematical and Computational Oncology (ISMCO).*

Computational analysis of complement inhibitor compstatin using molecular dynamics
Devaurs, D., Antunes, D. A. & Kavraki, L. E., 12 Aug 2020, In: Journal of Molecular Modeling. 26, 9, 9 p., 231.

HLA-Arena: a customizable environment for the structural modeling and analysis of peptide-HLA complexes for cancer immunotherapy
Antunes, D. A., Abella, J. R., Hall-Swan, S., Devaurs, D., Conev, A., Moll, M., Lizée, G. & Kavraki, L. E., 15 Jul 2020, In: JCO Clinical Cancer Informatics. 4, p. 623-636 14 p.

A robotics-inspired screening algorithm for molecular caging prediction
Kravchenko, O., Varava, A., Pokorny, F. T., Devaurs, D., Kavraki, L. E. & Kragic, D., 23 Mar 2020, In: Journal of Chemical Information and Modeling. 60, 3, p. 1302-1316 15 p.

Using parallelized incremental meta-docking can solve the conformational sampling issue when docking large ligands to proteins
Devaurs, D., Antunes, D. A., Hall-Swan, S., Mitchell, N., Moll, M., Lizée, G. & Kavraki, L. E., 5 Sept 2019, In: BMC Molecular and Cell Biology. 20, 1, 15 p., 42.

HLA-Arena: Structural modeling/analysis of peptide-HLA complexes
Devaurs, D. (Developer), 2019

Structure-based methods for binding mode and binding affinity prediction for peptide-MHC complexes
Antunes, D. A., Abella, J. R., Devaurs, D., Rigo, M. M. & Kavraki, L. E., 1 Dec 2018, In: Current Topics in Medicinal Chemistry. 18, 26, p. 2239-2255 17 p.

Revealing unknown protein structures using computational conformational sampling guided by experimental hydrogen-exchange data
Devaurs, D., Antunes, D. A. & Kavraki, L. E., 31 Oct 2018, In: International Journal of Molecular Sciences. 19, 11, 13 p., 3406.

Native state of complement protein C3d analysed via hydrogen exchange and conformational sampling
Devaurs, D., Papanastasiou, M., Antunes, D. A., Abella, J. R., Moll, M., Ricklin, D., Lambris, J. D. & Kavraki, L. E., 28 Mar 2018, In: International Journal of Computational Biology and Drug Design. 11, 1-2

General prediction of peptide-MHC binding modes using incremental docking: a proof of concept
Antunes, D. A., Devaurs, D., Moll, M., Lizée, G. & Kavraki, L. E., 12 Mar 2018, In: Scientific Reports. 8, 13 p., 4327.

DINC 2.0: a new protein-peptide docking webserver using an incremental approach
Antunes, D. A., Moll, M., Devaurs, D., Jackson, K. R., Lizée, G. & Kavraki, L. E., 1 Nov 2017, In: Cancer Research. 77, 21 , p. e55-e57 3 p.

Coarse-grained conformational sampling of protein structure improves the fit to experimental hydrogen-exchange data
Devaurs, D., Antunes, D. A., Papanastasiou, M., Moll, M., Ricklin, D., Lambris, J. D. & Kavraki, L. E., 10 Mar 2017, In: Frontiers in Molecular Biosciences. 4, 14 p., 13.

Defining low-dimensional projections to guide protein conformational sampling
Novinskaya, A., Devaurs, D., Moll, M. & Kavraki, L. E., 1 Jan 2017, In: Journal of Computational Biology. 24, 1, p. 79-89 11 p.

DINC: Docking INCrementally (molecular docking for large ligands)
Devaurs, D. (Developer), 2017

Optimal path planning in complex cost spaces with sampling-based algorithms
Devaurs, D., Siméon, T. & Cortés, J., 1 Apr 2016, In: IEEE Transactions on Automation Science and Engineering. 13, 2, p. 415-424 10 p.

Improving protein conformational sampling by using guiding projections
Novinskaya, A., Devaurs, D., Moll, M. & Kavraki, L. E., 17 Dec 2015, *2015 IEEE International Conference on Bioinformatics and Biomedicine (BIBM).* Schapranow, L. M., Zhou, J., Hu, X. T., Ma, B., Rajasekaran, S., Miyano, S., Yoo, I., Pierce, B., Shehu, A., Gombar, V. K., Chen, B., Pai, V. & Huan, J. (eds.). Piscataway, NJ: IEEE, p. 1272-1279 8 p. 7359863

Understanding the challenges of protein flexibility in drug design
Antunes, D. A., Devaurs, D. & Kavraki, L. E., 2 Dec 2015, In: Expert Opinion on Drug Discovery. 10, 12, p. 1301-1313 13 p.

Characterizing energy landscapes of peptides using a combination of stochastic algorithms
Devaurs, D., Molloy, K., Vaisset, M., Shehu, A., Siméon, T. & Cortés, J., 1 Jul 2015, In: IEEE Transactions on NanoBioscience . 14, 5, p. 545-552 8 p.

Sampling-based methods for a full characterization of energy landscapes of small peptides
Devaurs, D., Shehu, A., Siméon, T. & Cortés, J., 15 Jan 2015, *2014 IEEE International Conference on Bioinformatics and Biomedicine (BIBM).* Zheng, H., Dubitzky, W., Hu, X., Hao, J.-K., Berrar, D., Cho, K.-H., Wang, Y. & Gilbert, D. (eds.). Piscataway, NJ: IEEE, p. 37-44 8 p.

Efficient sampling-based approaches to optimal path planning in complex cost spaces
Devaurs, D., Siméon, T. & Cortés, J., 1 Jan 2015, *Algorithmic Foundations of Robotics - Selected Contributions of the 11th International Workshop on the Algorithmic Foundations of Robotics, WAFR 2014.* Levent Akin, H., Amato, N. M., Isler, V. & Stappen, A. F. (eds.). Cham, Switzerland: Springer, p. 143-159 17 p. (Springer Tracts in Advanced Robotics; vol. 107).

A multi-tree extension of the transition-based RRT: application to ordering-and-pathfinding problems in continuous cost spaces
Devaurs, D., Siméon, T. & Cortés, J., 6 Nov 2014, *2014 IEEE/RSJ International Conference on Intelligent Robots and Systems.* Piscataway, NJ: IEEE, p. 2991-2996 6 p. 6942975. (IEEE International Conference on Intelligent Robots and Systems).

Extensions of Sampling-based Approaches to Path Planning in Complex Cost Spaces: Applications to Robotics and Structural Biology
Devaurs, D., 10 Oct 2014

MoMA LigPath: Molecular Motion Algorithms (robotics-inspired molecular modeling)
Devaurs, D. (Developer), 2014

Enhancing the transition-based RRT to deal with complex cost spaces
Devaurs, D., Siméon, T. & Cortés, J., 17 Oct 2013, *2013 IEEE International Conference on Robotics and Automation.* Piscataway, NJ: IEEE, p. 4120-4125 6 p. 6631158. (Proceedings - IEEE International Conference on Robotics and Automation).

A motion planning approach to 6-D manipulation with aerial towed-cable systems
Manubens, M., Devaurs, D., Ros, L. & Cortés, J., 20 Sept 2013. 7 p.

A multi-tree approach to compute transition paths on energy landscapes
Devaurs, D., Vaisset, M., Siméon, T. & Cortés, J., 14 Jul 2013, *Artificial Intelligence and Robotics Methods in Computational Biology - Papers from the 2013 AAAI Workshop, Technical Report.* California : AI Access Foundation, p. 8-13 6 p.

MoMA-LigPath: a web server to simulate protein-ligand unbinding
Devaurs, D., Bouard, L., Vaisset, M., Zanon, C., Al-Bluwi, I., Iehl, R., Siméon, T. & Cortés, J., 1 Jul 2013, In: Nucleic Acids Research. 41, W1, p. W297-W302 6 p.

Motion planning for 6-D manipulation with aerial towed-cable systems
Manubens, M., Devaurs, D., Ros, L. & Cortés, J., 28 Jun 2013. 8 p.

Parallelizing RRT on large-scale distributed-memory architectures
Devaurs, D., Siméon, T. & Cortés, J., 1 Apr 2013, In: IEEE Transactions on Robotics. 29, 2, p. 571-579 9 p.

Exploiting the user interaction context for automatic task detection
Devaurs, D., Rath, A. S. & Lindstaedt, S. N., 6 Feb 2012, In: Applied Artificial Intelligence. 26, 1-2, p. 58-80 23 p.

Parallelizing RRT on distributed-memory architectures
Devaurs, D., Siméon, T. & Cortés, J., 18 Aug 2011, *2011 IEEE International Conference on Robotics and Automation.* Piscataway, NJ: IEEE, p. 2261-2266 6 p. 5979751. (Proceedings - IEEE International Conference on Robotics and Automation).

Automatic detection of accommodation steps as an indicator of knowledge maturing
Moskaliuk, J., Rath, A., Devaurs, D., Weber, N., Lindstaedt, S., Kimmerle, J. & Cress, U., 1 May 2011, In: Interacting with Computers. 23, 3, p. 247-255 9 p.

An ontology-based approach for detecting knowledge intensive tasks
Rath, A. S., Devaurs, D. & Lindstaedt, S. N., 1 Feb 2011, In: Journal of Digital Information Management. 9, 1, p. 9-18 10 p.

Studying the factors influencing automatic user task detection on the computer desktop
Rath, A. S., Devaurs, D. & Lindstaedt, S. N., 1 Sept 2010, *Sustaining TEL: From Innovation to Learning and Practice - 5th European Conference on Technology Enhanced Learning, EC-TEL 2010, Proceedings.* Cham, Switzerland: Springer, p.

292-307 16 p. (Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics); vol. 6383 LNCS).

Species abundance patterns in an ecosystem simulation studied through Fisher's logseries
Devaurs, D. & Gras, R., 1 Jan 2010, In: Simulation Modelling Practice and Theory. 18, 1, p. 100-123 24 p.

An individual-based evolving predator-prey ecosystem simulation using a fuzzy cognitive map as the behavior model
Gras, R., Devaurs, D., Wozniak, A. & Aspinall, A., 1 Oct 2009, In: Artificial Life. 15, 4, p. 423-463 41 p.

Machine learning based work task classification
Granitzer, M., Rath, A. S., Kröll, M., Seifert, C., Ipsmiller, D., Devaurs, D., Weber, N. & Lindstaedt, S., 1 Oct 2009, In: Journal of Digital Information Management. 7, 5, p. 305-312 8 p.

Contextualized knowledge services for personalized learner support
Rath, A. S., Devaurs, D. & Lindstaedt, S. N., 29 Sept 2009.

Detecting real user tasks by training on laboratory contextual attention metadata
Rath, A. S., Devaurs, D. & Lindstaedt, S. N., 28 Sept 2009, *INFORMATIK 2009 - Im Focus das Leben, Beitrage der 39. Jahrestagung der Gesellschaft fur Informatik e.V. (GI).* Bonn, Germany, p. 1645-1653 9 p.

KnowSe: fostering user interaction context awareness
Rath, A. S., Devaurs, D. & Lindstaedt, S. N., 7 Sept 2009.

UICO: an ontology-based user interaction context model for automatic task detection on the computer desktop
Rath, A. S., Devaurs, D. & Lindstaedt, S. N., 1 Jun 2009, *Proceedings of the 1st Workshop on Context, Information and Ontologies, CIAO 2009.* New York, NY, 10 p. 8

Timed transition discovery from Web service conversation logs
Devaurs, D., Musaraj, K., De Marchi, F. & Hacid, M.-S., 20 Jun 2008, In: CEUR Workshop Proceedings. 344, p. 53-56 4 p.

Caractérisation des transitions temporisées dans les logs de conversation de services Web
Devaurs, D., de Marchi, F. & Hacid, M.-S., 26 Jan 2007, *Extraction et Gestion des Connaissances (EGC): Volumes I et II.* Noirhomme-Fraiture, M. & Venturini, G. (eds.). Toulouse, France, p. 45-56 12 p.

Génération de bases de transactions synthétiques : vers la prise en compte des bordures
Devaurs, D. & De Marchi, F., 20 Oct 2005, p. 119-133. 15 p.

Prizes

Finalist in the STEM for BRITAIN poster competition
Devaurs, D. (Recipient), 6 Mar 2023

IGC travel grant
Devaurs, D. (Recipient), May 2022

SULSA ECR prize
Devaurs, D. (Recipient), Feb 2022

9th ACM-BCB conference poster award
Devaurs, D. (Recipient), Sept 2018

4th annual Smalley-Curl Institute summer research colloquium's poster award
Devaurs, D. (Recipient), Aug 2018

23rd Sealy Center for Structural Biology and Molecular Biophysics symposium's poster award
Devaurs, D. (Recipient), Apr 2018

27th annual Keck Center Research conference's poster award
Devaurs, D. (Recipient), Oct 2017

22nd Sealy Center for Structural Biology and Molecular Biophysics symposium's poster award
Devaurs, D. (Recipient), May 2017

21st Sealy Center for Structural Biology and Molecular Biophysics symposium's poster award
Devaurs, D. (Recipient), Apr 2016

Léopold Escande Ph.D. award
Devaurs, D. (Recipient), Dec 2014

IEEE ICRA '13 student travel grant
Devaurs, D. (Recipient), May 2013

Activities

AlphaSense Expert Insights
Devaurs, D. (Advisor)
Nov 2024 → …

Archives of Biochemistry and Biophysics (Journal)
Devaurs, D. (Editorial board member)
Oct 2024 → …

IEEE Access (Journal)
Devaurs, D. (Peer reviewer)
Oct 2024

A robotics-inspired screening algorithm for high-throughput molecular caging prediction
Devaurs, D. (Speaker)
5 Sept 2024

ACS Chemical Neuroscience (Journal)
Devaurs, D. (Peer reviewer)
Sept 2024

Industrial Biotechnology Innovation Centre (IBioIC) (External organisation)
Devaurs, D. (Member)
Sept 2024 → …

Heliyon (Journal)
Devaurs, D. (Peer reviewer)
Aug 2024

Chemical Reviews (Journal)
Devaurs, D. (Peer reviewer)

Jul 2024

University Of Strathclyde (Organisational unit)
Devaurs, D. (Member)
Jul 2024 → …

A tale of two strategies to efficiently explore the conformational space of molecular systems
Devaurs, D. (Speaker)
Jun 2024

Biochimica et Biophysica Acta - General Subjects (Journal)
Devaurs, D. (Peer reviewer)
Jun 2024

Biomolecules (Journal)
Devaurs, D. (Editorial board member)
Jun 2024 → …

Outcomes and impact of the early career researcher (ECR) prize
Devaurs, D. (Speaker)
May 2024

A Rosetta-based pipeline for molecular modelling guided by experimental HDX-MS data
Devaurs, D. (Speaker)
Apr 2024

Studying protein structure using experimental HDX-MS data and multi-resolution conformational sampling
Devaurs, D. (Speaker)
Mar 2024

A tale of two AI-based strategies for molecular studies
Devaurs, D. (Speaker)
Nov 2023

Studying protein structure using experimental HDX-MS data and multi-resolution conformational sampling
Devaurs, D. (Speaker)
Nov 2023

Predicting accurate binding modes for peptide-HLA complexes using parallelized incremental meta-docking
Devaurs, D. (Speaker)
Oct 2023

Biotechnology and Biological Sciences Research Council (External organisation)
Devaurs, D. (Advisor)
Sept 2023

Studying protein structure using experimental HDX-MS data and multi-resolution conformational sampling
Devaurs, D. (Speaker)
Sept 2023

Association for Computing Machinery (External organisation)
Devaurs, D. (Member)
Jul 2023 → …

Improving the coverage of deep mutational scanning using machine learning
Devaurs, D. (Speaker)
Jul 2023

Improving the coverage of deep mutational scanning using machine learning
Devaurs, D. (Speaker)
Jul 2023

Predicting accurate binding modes for peptide-HLA complexes using parallelized incremental meta-docking
Devaurs, D. (Speaker)
Jul 2023

A tale of two strategies to efficiently explore the conformational space of molecular systems
Devaurs, D. (Speaker)
Jun 2023

A tale of two strategies to efficiently explore the conformational space of molecular systems
Devaurs, D. (Speaker)
Jun 2023

A tale of two strategies to efficiently explore the conformational space of molecular systems
Devaurs, D. (Speaker)
Jun 2023

A tale of two strategies to efficiently explore the conformational space of molecular systems
Devaurs, D. (Speaker)
May 2023

A tale of two strategies to efficiently explore the conformational space of molecular systems
Devaurs, D. (Speaker)
Apr 2023

Voice of Young Science (External organisation)
Devaurs, D. (Member)
Apr 2023 → May 2024

Interpreting the health impact of genetic variation via deep mutational scanning and machine learning
Devaurs, D. (Speaker)
6 Mar 2023

Making deep mutational scanning actionable to interpret protein variant effects
Devaurs, D. (Speaker)
6 Mar 2023

A tale of two strategies to efficiently explore the conformational space of molecular systems
Devaurs, D. (Speaker)
Mar 2023

A tale of two strategies to efficiently explore the conformational space of molecular systems
Devaurs, D. (Speaker)
Mar 2023

A tale of two strategies to efficiently explore the conformational space of molecular systems
Devaurs, D. (Speaker)
Nov 2022

A tale of two strategies to efficiently explore the conformational space of molecular systems
Devaurs, D. (Speaker)
Oct 2022

A tale of two strategies to efficiently explore the conformational space of molecular systems
Devaurs, D. (Speaker)
Oct 2022

BMC Bioinformatics (Journal)
Devaurs, D. (Editorial board member)
Oct 2022 → …

Frontiers in Molecular Biosciences (Journal)
Devaurs, D. (Editorial board member)
Jun 2022 → Sept 2024

Computational modeling of molecular structures guided by experimental HDX-MS data
Devaurs, D. (Speaker)
Apr 2022

American Chemical Society (External organisation)
Devaurs, D. (Member)
Jan 2022 → Dec 2022

Lessons learned from modelling data, robots and molecules
Devaurs, D. (Speaker)
Nov 2021

Studying protein structure using HDX-MS and multi-resolution conformational sampling
Devaurs, D. (Speaker)
Sept 2021

International Society for HDX-MS (External organisation)
Devaurs, D. (Member)
Aug 2021 → …

Biochemistry and Biophysics Reports (Journal)
Devaurs, D. (Editorial board member)
Jan 2021 → Jan 2023

European Conference on Computational Biology (Event)
Devaurs, D. (Peer reviewer)
Jan 2021 → Jul 2021

Intelligent Systems for Molecular Biology (Event)
Devaurs, D. (Peer reviewer)
Jan 2021 → Jul 2021

Frontiers in Bioengineering and Biotechnology (Journal)
Devaurs, D. (Peer reviewer)
2021 → 2024

Frontiers in Bioinformatics (Journal)
Devaurs, D. (Peer reviewer)
2021 → 2024

Frontiers in Drug Discovery (Journal)
Devaurs, D. (Peer reviewer)
2021 → 2024

Frontiers in Molecular Biosciences (Journal)
Devaurs, D. (Peer reviewer)
2021 → 2024

Antibiotics (Journal)
Devaurs, D. (Guest editor)
Oct 2020 → Oct 2021

Lessons learned from modelling data, robots and molecules
Devaurs, D. (Speaker)
Apr 2020

Modeling intrinsically disordered regions in proteins
Devaurs, D. (Speaker)
Jan 2020

Antibiotics (Journal)
Devaurs, D. (Peer reviewer)
2020 → 2024

Efficient strategies to explore the conformational space of proteins and molecular complexes
Devaurs, D. (Speaker)
Nov 2019

Guiding protein conformational sampling with experimental hydrogen exchange data to uncover unknown structures
Devaurs, D. (Speaker)
Nov 2019

Studying protein structure through hydrogen exchange and coarse-grained conformational sampling
Devaurs, D. (Speaker)
Nov 2019

Efficient strategies to explore the conformational space of proteins and molecular complexes
Devaurs, D. (Speaker)
Sept 2019

Efficient strategies to explore the conformational space of proteins and molecular complexes
Devaurs, D. (Speaker)
Sept 2019

Current Proteomics (Journal)
Devaurs, D. (Editorial board member)
Jan 2019 → Jan 2021

Biophysical Reviews (Journal)
Devaurs, D. (Editorial board member)
Nov 2018 → May 2024

International Conference on Bioinformatics and Computational Biology (Event)
Devaurs, D. (Peer reviewer)
Oct 2018 → Mar 2019

Guiding protein conformational sampling with experimental hydrogen exchange data to uncover unknown structures
Devaurs, D. (Speaker)
Sept 2018

Efficiently exploring the conformational space of proteins and molecular complexes
Devaurs, D. (Speaker)
Aug 2018

General prediction of peptide-MHC binding modes using incremental docking: A proof of concept
Devaurs, D. (Speaker)
Aug 2018

Guiding protein conformational sampling with hydrogen exchange data to uncover unknown structures
Devaurs, D. (Speaker)
Aug 2018

ACM SIGBIO (External organisation)
Devaurs, D. (Member)
Jul 2018 → Jun 2019

Predicting binding modes of peptide-HLA complexes with molecular docking
Devaurs, D. (Speaker)
Apr 2018

International Conference on Digital Information Management (Event)
Devaurs, D. (Peer reviewer)
Mar 2018 → Sept 2018

Predicting binding modes of peptide-HLA complexes with molecular docking
Devaurs, D. (Speaker)
Nov 2017

Predicting binding modes of peptide-HLA complexes with molecular docking
Devaurs, D. (Speaker)
Oct 2017

Studying protein structure through hydrogen exchange and conformational sampling
Devaurs, D. (Speaker)
Aug 2017

ACM Int. Conference on Bioinformatics, Computational Biology, and Health Informatics (Event)
Devaurs, D. (Peer reviewer)
Jan 2017 → Aug 2017

Native state of complement protein C3d analyzed via hydrogen exchange and conformational sampling
Devaurs, D. (Speaker)
Dec 2016

Czech Science Foundation (External organisation)
Devaurs, D. (Advisor)
Mar 2016

Efficient sampling-based approaches to optimal path planning in complex cost spaces
Devaurs, D. (Speaker)
Aug 2014

MoMA-LigPath: A web server to simulate protein-ligand unbinding
Devaurs, D. (Speaker)
Jul 2013

Institute of Electrical and Electronics Engineers (External organisation)
Devaurs, D. (Member)
Jun 2013 → May 2014

Teaching Interests

Higher education teaching:

Bioinformatics

Artificial intelligence
Past academic advising (University of Edinburgh):

Zihan Kong, M.Sc. in bioinformatics (2023)

Tianyu Zhao, M.Sc. in bioinformatics (2023)

Xinyu Liu, M.Sc.R in integrative biomedical sciences (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)
Past academic advising (Rice University):

Anja Conev, B.Sc. in computer science (2018)

Nicole Mitchell, B.Sc. in computer science (2018)

Elizabeth Palmi, B.Sc. in computer science (2018)

Stephen Price, B.Sc. in computer science (2018)

Sarah Hall-Swan, B.Sc. in computer science (2017)

Angela Hoch, B.Sc. in computer science (2017)

Yovahn Hoole, B.Sc. in computer science (2017)

Research Interests

In the past two decades, my research has focused on the computational modelling, simulation and analysis of complex physical systems, both in robotics and structural biology. At the algorithmic level, simulating mobile or flexible systems (such as robots and molecules) requires exploring a high-dimensional space: the space of all the possible states of the system. My work has involved developing efficient algorithms and heuristics to address this challenge.
During my PhD at LAAS-CNRS, I developed novel extensions of sampling-based path planning algorithms and created the concept of optimal path planning in a cost space (**section 1**). As a post-doctoral researcher at Rice University, I developed computational methods to efficiently explore the conformational space of proteins using experimental data as a

guide (**section 2**), and to incrementally dock large ligands to protein receptors (**section 3**). I also helped develop a robotics-inspired method to predict whether a molecule could cage another one (**section 4**).
As a research fellow at the University of Edinburgh, I worked on several quantitative biomedical research projects:

modelling the interaction network of cell-adhesion proteins in cancer cells

analysing time series of white blood cell data from the Generation Scotland cohort

improving the coverage of deep mutational scanning experiments using machine learning.
The main application of my current research is to produce clinical interpretations of genetic mutations in people, using machine learning and data from deep mutational scanning experiments. This research is of great significance, as deep mutational scanning is a promising technique in the quest for personalised medicine. Indeed, being able to derive the functional effects of rare mutations in important genes would be a crucial breakthrough for medical practice.

1. Optimal path planning in cost spaces with sampling-based algorithms
During my PhD, I developed novel extensions of sampling-based path planning algorithms. Despite their conceptual simplicity, these algorithms can efficiently explore a high-dimensional space in a probabilistic manner and build a graph representing the topology of this space. They had traditionally been used in simple robotic applications to find feasible (i.e., collision-free) paths, without considering path quality. However, many applications require to compute high-quality (i.e., low-cost) paths or even optimal paths, in the context of cost-space path planning or optimal path planning. To deal with ever more complex applications, I proposed the following contributions:

I enhanced a cost-space path planning algorithm, called Transition-based Rapidly-exploring Random Tree (T-RRT), by creating bidirectional and multiple-tree variants. I also proposed three parallel versions of T-RRT-like algorithms to improve scalability. Then, I used these algorithms to plan for 6-dimensional manipulation with a towed-cable system involving three aerial robots (in simulation).

I combined the paradigms of cost-space path planning and optimal path planning to create the concept of optimal path planning in a cost space. In this context, I developed two new algorithms (T-RRT* and Anytime T-RRT) for the Move3D robotic platform and the MoMA molecular modelling library. I also showed that both algorithms were probabilistically complete and asymptotically optimal. I applied them to the planning of industrial inspection tasks performed by flying robots (in simulation) and to the exploration of the energy landscape of small peptides.
Main references:

Optimal path planning in complex cost spaces with sampling-based algorithms; IEEE Transactions on Automation Science and Engineering; 2016; DOI: 10.1109/TASE.2015.2487881

MoMA-LigPath: A web server to simulate protein-ligand unbinding; Nucleic Acids Research; 2013; DOI: 10.1093/nar/gkt380

Parallelizing RRT on large-scale distributed-memory architectures; IEEE Transactions on Robotics; 2013; DOI: 10.1109/TRO.2013.2239571

2. Protein structural sampling guided by experimental hydrogen-exchange data
Gathering experimental data about a protein’s three-dimensional structure allows understanding its function and possible dysfunctions. In addition, computational techniques exist to explore a protein's conformational space, i.e., the space of all possible states (or conformations) of the protein. However, experimentally observing and computationally modelling large proteins remain critical challenges for structural biology. To address this issue, I developed a novel approach integrating an experimental technique and a computational method to analyse large proteins. I studied how the computational exploration of a protein’s conformational space could be guided by sparse structural information, such as the experimental data obtained through hydrogen exchange (HX) monitoring. For that, I extended a computational framework called Structured Intuitive Move Selector (SIMS) performing coarse-grained structural sampling, i.e., in which not all perturbations (or moves) applied to protein conformations consider a protein in its full atomistic resolution.
SIMS combines robotics-inspired structural sampling algorithms with the popular Rosetta library for protein modelling. I published three applications of my method:

I showed that my method yields a better fit between HX data and computationally-generated protein conformations than other HX-guided conformational sampling methods.

I showed that I could analyse the inherent variability of a protein's native state (i.e., its equilibrium state in solution).

I showed that I could generate structural models for protein states described only by HX data.

Main references:

Computational modeling of molecular structures guided by hydrogen-exchange data; Journal of the American Society for Mass Spectrometry; 2022; DOI: 10.1021/jasms.1c00328

Revealing unknown protein structures using computational conformational sampling guided by experimental hydrogen-exchange data; International Journal of Molecular Sciences; 2018; DOI: 10.3390/ijms19113406

Coarse-grained conformational sampling of protein structure improves the fit to experimental hydrogen-exchange data; Frontiers in Molecular Biosciences; 2017; DOI: 10.3389/fmolb.2017.00013

3. Molecular docking of large ligands to protein receptors

Although there is a variety of software for the molecular docking of protein-ligand complexes, most docking tools can only deal with small drug-like ligands. The docking of large ligands, including peptides, is still considered a challenge in computational structural biology. To address this issue, I developed a molecular docking tool, called DINC, specifically aimed at dealing with large ligands, following a parallelized incremental meta-docking approach. DINC is a meta-docking tool in the sense that it uses existing docking software at its core. Following the divide-and-conquer paradigm, it was conceived as an incremental method that iteratively docks larger and larger overlapping fragments of a ligand in the protein's binding site. This research was motivated by the study of molecular complexes important in cancer immunotherapy.

I extended this approach to address a limitation of DINC and numerous other docking tools: the fact that they do not account for receptor flexibility when docking a flexible ligand. Because of COVID-19, my collaborators and I chose to specifically implement a computational tool for ensemble docking with SARS-CoV-2 proteins. We extracted representative ensembles of protein conformations from the Protein Data Bank and from computer simulations. Twelve pre-computed ensembles of SARS-CoV-2 protein conformations are available for ensemble docking via a user-friendly webserver called DINC-COVID. We validated DINC-COVID using tested inhibitors of two SARS-CoV-2 proteins, obtaining good correlations between docking-derived binding energies and experimental binding affinities.

Main references:

DINC-COVID: A webserver for ensemble docking with flexible SARS-CoV-2 proteins; Computers in Biology and Medicine; 2021; DOI: 10.1016/j.compbiomed.2021.104943

Using parallelized incremental meta-docking can solve the conformational sampling issue when docking large ligands to proteins; BMC Molecular and Cell Biology; 2019; DOI: 10.1186/s12860-019-0218-z

General prediction of peptide-MHC binding modes using incremental docking: A proof of concept; Scientific Reports; 2018; DOI: 10.1038/s41598-018-22173-4

4. Robotics-inspired screening for molecular caging prediction

A molecular caging complex is defined as a pair of molecules in which a so-called host (or cage) features an internal cavity that can enclose a so-called guest, preventing its escape. In synthetic biochemistry, a host molecule is usually created with dynamic covalent bonds allowing its self-assembly around a guest molecule and its later disassembly in response to a specific stimulus (such as temperature, pH, or light). This paradigm has produced exciting biomedical applications, for example in targeted drug delivery, virus trapping, or medical imaging. Despite its promises, the use of molecular caging complexes remains challenging, with the discovery or synthesis of host molecules being the main bottleneck. There is thus a need for computational screening methods that can predict whether a given pair of molecules form a caging complex.

We proposed such a method, based on a caging verification algorithm that was initially designed for applications in robotic manipulation. We tested our algorithm on three pairs of molecules that were previously described in a pioneering work on molecular caging complexes and found that our results were fully consistent with previously reported ones. We also performed a screening experiment on a data set consisting of 46 hosts and four guests and used our algorithm to predict which pairs were likely to form caging complexes. Our method is computationally efficient and can be integrated into a screening pipeline to complement experimental techniques. This is important because the possibility of performing computational screening studies would propel biomedical applications even further and deliver substantial impact.

Main reference:

A robotics-inspired screening algorithm for molecular caging prediction; Journal of Chemical Information and Modeling; 2020; DOI: 10.1021/acs.jcim.9b00945