Kieran Didi, Overview of publications, conference presentations, software, and teaching

Publications

- Flexible Small-Molecule Design and Optimization via Equivariant Diffusion Models, ILCR 2023 MLDD Workshop, 03/2023
- Accessible genomics at scale: developing a cloud-native platform to detect foreign DNA insertions, under review, 03/2023
- High Resolution Biomolecular Condensate Phase Diagrams with a Combinatorial Microdroplet Platform, Nature Communications, 12/2022
 - Developed screening system and bioinformatic analysis for protein analysis, especially LLPS behaviour of intrinsically disordered proteins and the effect on structure/function
- On How AI needs to Change to Advance the Science of Drug Discovery, <u>arxiv</u>, 12/2022
- Generative Models in Bioinformatics, invited book chapter in Encyclopedia of Bioinformatics and Computational Biology, under review, 01/2023

Conference Presentations

- Accessible AMR-detection tools for clinicians via cloud-based bioinformatics (oral presentation), Clinical Informatics Symposium Melbourne (Australia), 12/2022
- sINSIDER: a cloud-native modular platform for kmer-based genomic analysis (oral presentation), ABACBS Conference Melbourne (Australia), 11/2022
- Moving bioinformatics to the cloud (keynote presentation), eSCAMPS Symposium Cambridge (UK), 09/2022
- Detecting DNA integration via HPC bioinformatics pipeline (poster), R&I Conference Sydney (Australia), 08/2022

Open-Source Software Contributions

- Terraform module for automated setup of EMR Serverless application (published on <u>Terraform registry</u>) including <u>detailed tutorial</u>, more than 600 downloads so far (<u>research background</u>)
- Web application to detect foreign DNA integrations quickly, example usages include hospitals
 for detection of antimicrobial resitances and clinical trials checking for integration events in
 gene therapy. Based on high-performance serverless architecture, source code <u>publicly</u>
 available
- <u>Multimodal Healthcare project</u> to integrate data from different sources (clinical notes, genomics, MRI scans, ...) to predict cardiovascular disease risk, part of FSDL course 2022
- Part of a team for a <u>Kaggle challenge</u> to predict protein stability based on sequence information
- Implement biologicial oracle for effect prediction of *in silico* generated biological sequences, part of the <u>DNA Diffusion project</u> at <u>OpenBioML research lab</u>

Teaching

- <u>Algorithms II</u>, supervising course on data structures and graph algorithms, Cambridge University, 01-03/2023
- MLOps with PyTorch Lightning and W&B, conceptualised and lecture workshop, ML Forum CSIRO Australia, 01/2023
- Python for Scientists, conceptualised and lectured course, Heidelberg University, 11/2022
- Python Best Practices, co-host of this workshop, Scientific Software Centre Heidelberg 11/2022
- <u>Deep Learning with PyTorch</u>, Lunch Time Python workshop, Scientific Software Centre Heidelberg, 10/2022

•	Python for Biochemists, 03/2022	conceptualised and lectured	course, Heidelberg University,