Travis P. Hesketh

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Senior Python software engineer with strengths in data engineering and backend development. Chemistry graduate, with a focus in computational chemistry and cheminformatics. Several years of research experience in academic and commercial settings. Currently based in Leeds.

Skills

- Python software development using both functional and object-oriented paradigms. Specific emphasis on clean, understandable, intuitive code.
- Cloud computing with AWS.
- Data manipulation using SQL (Postgres-flavoured and Spark) PySpark, pandas and numpy.
- API development with FastAPI/Flask, using both relational and NoSQL data stores.
- Unit testing with pytest and effective code documentation using pydoc and Sphinx/autodoc.

Education

Chemistry (Professional Experience), *University of Strathclyde*, 2014 – 2018

Bachelor of Science, First Class Honours

Employment

Senior Software Developer, *Aire Logic Ltd.*, July 2021 – Present

Software Developer, *Aire Logic Ltd.*, July 2020 – July 2021

Employed as a backend Python engineer to work as a consultant in the healthcare sector.

- Heavily involved in the recruitment process, interviewing and assessing prospective staff.
- Key technical contributor to tenders on NHS Digital's £800m Digital Capability for Health framework.

Data Engineer (Contract), *NHS Digital (Open Data and Dashboards)*, September 2020 – September 2021

Supported key aspects of NHS Digital's COVID response: data reporting for COVID statistics. Technologies: Athena, Databricks, EC2, Python, S3, SQL, Tableau. On contract from Aire Logic.

- Solved blocking deployment issues for NHS Digital's Coronavirus in Your Area dashboard.

- Planned, instigated and implemented a cloud migration for key data pipelines, increasing security, observability & monitoring and decreasing both cost & complexity.
- Supported key private dashboards used by DHSC and local government to monitor pandemic progression and prioritise resource allocation.
- Introduced automated testing to ensure data quality and improve reliability.
- Supported other teams to expand use of best practices and facilitate knowledge transfer.

Postgraduate Researcher, *University of Strathclyde*, October 2018 – June 2020

Conducted PhD-level research in computational chemistry using molecular dynamics to investigate bioinspired materials. Technologies: Python, OpenMM, scikit-learn.

- Made extensive use of Python workflows for simulation and analysis.
- Mentored several students, teaching Linux and Python, and wrote workflow tutorials.
- Worked as a tutor and lab demonstrator, responsible for groups of up to 50 students.
- Collaborated internationally with a New York-based group.

Industrial Placement, *Optibrium Ltd.*, July 2017 – July 2018

Worked in cheminformatics as part of the computational chemistry team, developing machine learning models to predict biological assay results. Technologies: Python, scikit-learn, SQL.

- Successfully developed models to predict inhibition of important drug antitargets, which are currently in use in the pharmaceutical industry.
- Designed and implemented filtering workflow in Python to aid in curation, which was presented at a leading international conference.

Publications

Hesketh, T., pygen-structures: A Python package to generate 3D molecular structures for simulations using the CHARMM forcefield, *J Open-Source Softw.*, 2020, 5(48), 2157, DOI:10.21105/joss.02157

Hesketh, T. and Tuttle, T., Steps Towards Understanding Water Responsiveness, poster presented at the *2019 ScotCHEM Computational Chemistry Symposium,* 26th June 2019. https://bit.ly/2K31fvU *Winner of the ScotCHEM Prize.*

Interests

Big fan of film and TV. Interested in open source software. Currently learning Rust. Enjoy being around and meeting new people, keeping up to date with current events, playing guitar, and sudoku puzzles. Vinyl collector, typography fan, and indoor climber.