David Wright

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About Me

I am a researcher and software engineer. My career in academia has provided me with a wide range of problem solving skills and experience running and maintaining IT infrastructure. I have also led small development teams and collaborated in large multi-national projects. I am now looking to challenge my self in an industrial setting.

Skills

Programming: Python, R

Molecular Simulation

Data Analysis

High Performance Computing

System Administration

Containerization: Docker, Singularity

Cloud: Kubernetes, Azure, AWS, Google

Programming: Fortran, C

References

Peter V. Coveney

p.v.coveney@ucl.ac.uk

Elizabeth Rodriguez

elizabeth.rodriguez@ucb.com

Experience

2016 - present **Research Associate** — **Centre for Computational Science, UCL**

- Develop molecular simulation and analysis approaches to predict the strength of small molecule binding to protein targets for drug discovery applications.
- Lead team of developers on BAC 2.0 tool designed to automate molecular simulations using multiple packages (GROMACS, NAMD, etc.) and HTBAC workflow management tool.
- Lead development of the EasyVVUQ tool to automate verification, validation and uncertainty quantification for high performance computing applications.
- Research representative on the UCL Research Data Repository project board.
- Supervision of Masters and Ph.D. students.
- Organization of the "Free Energy Calculations from Molecular Simulation" workshop - in collaboration with the CompBioMed and BioExcel projects.
- Named investigator on the INSPIRE project (supported by the US department of INCITE program) combining molecular dynamics and machine learning to study cancer drug resistance.
- Contributing to writing of grant proposals, including those successfully approved for multimillion € CompBioMed2 and VECMA EU projects.

2017 - present **Chief Scientific Officer** — **EnsembleMD**

- Development and deployment of cloud based (SaaS) molecular simulation tools for multiple providers.
- Structural modelling of antibodies from small angle scattering data for pharmaceutical companies.

2013 - 2016 **Research Associate** — **Structural Immunology Group, UCL**

- Modelling and simulation of antibody and other immune system proteins with the aim of understanding structural data.
- Lead developer of SCT, a Python package for the comparison of atomistic models to small angle scattering data.
- Contributed to several structural modelling packages within the CCP-SAS project (SASSIE, SasMol, PDBRx, PDBScan) and a common web interface for them (made available at).

2011 - 2013 **Research Associate** — **Centre for Computational Science, UCL**

- Use of molecular dynamics simulations to understand the influence of protein mutations on drug binding.
- Administration of network of 12 desktop machines and small (20 node) cluster.
- Liaison with experimental groups in multinational medical and experimental project (CHAIN).

2010 - 2011 **Biomedical Simulation Consultant**

- Creation and testing of high performance computing workflow tools for Louisiana State University.
- Development (C and Fortran) of advanced simulation software for Fujitsu Laboratories of Europe.

Education

2011	**Ph.D., Chemistry** Molecular Dynamics Simulation of Drug Resistance in HIV-1 Protease and Reverse Transcriptase *Advisor: Prof. Peter V. Coveney*	**UCL**
2006	**M Res (Distinction), CoMPLEX** Modelling Biological Complexity	**UCL**
2003	**M Phys (1st), Computational Physics**	**University of York**

Publications

A full list of my publications can be found on **Google scholar**.