# **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

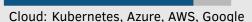
Molecular Simulation

Data Analysis

**High Performance Computing** 

System Administration

Containerization: Docker, Singularity



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 UCL Molecular Dynamics Simulation of Drug Resistance in HIV-1 Protease and Reverse Transcriptase Advisor: Prof. Peter V. Coveney 2006 UCL

M Res (Distinction), CoMPLEX **Modelling Biological Complexity** 

University of York 2003 M Phys (1st), Computational Physics

### **Publications**

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