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, Fortran, C

Molecular Simulation

Presentation Delivery

Project Management

Data Analysis

High Performance Computing

System Administration

Containerization: Docker, Singularity

Cloud: Kubernetes, Azure, AWS, Google

References

Available upon request

Experience

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

- Develop molecular simulation approaches to predict the strength of small molecule binding to protein targets for drug discovery applications.
- Process and analyze large quantities of simulation, experimental and clinical data.
- Lead team of developers on BAC 2.0 tool designed to automate molecular simulations using multiple applications 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, involving collating and communicating user needs and providing feedback on project design and implementation.
- Contribute to reviews and panels informing strategic decisions in the European HPC (through the EXDCI project and PRACE scientific steering committee).
- Supervision of Masters and Ph.D. students, including both day to day direction of research, deadline management and coordination with primary supervisors.
- 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 the CompBioMed2 (€8m) and VECMA (€4m) 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.
- Liaise with clients to determine their requirements and design solutions to fulfill them.

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

- Modelling and simulation of antibodies 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.
- Head UK developer within the joint UK-US project CCP-SAS. Developed structural modelling packages (PDBRx, PDBScan), and contributed to underlying libraries (SASSIE, SasMol) and a common web interface for all project software (made available at sassie-web.chem.utk.edu).
- Trained users in the use of CCP-SAS tools, including teaching at a summer school at ILL in Grenoble, France.

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

- Use of molecular dynamics simulations to understand the influence of protein mutations on drug binding.
- Administrator for network of 12 desktop machines and small 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 **M Res (Distinction), CoMPLEX** **UCL**
Modelling Biological Complexity

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

Publications and Presentations

I have published 29 articles in leading journals and conference proceedings. A full list of my publications can be found on **Google scholar**.

I have presented work at major conferences such as the Biophysical Society Annual Meeting, in 2012, 2013 and 2015, and International Supercomputing Conference (ISC) in 2018.