Hannes **Vandecasteele**, PhD

Computational Scientist • Applied Mathematician

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Computational scientist specializing in numerical algorithms, scientific machine learning, and computational drug design. Currently a postdoctoral researcher at Johns Hopkins University, developing machine learning-based surrogate models for numerical algorithms in computational chemistry. Previously worked on Markov chain Monte Carlo methods for multiscale molecular dynamics with extensive experience in high-performance computing, scientific software development, and probabilistic modeling. I have a track record of over 10 years in computational science, spanning academia and industry, including time as a software engineer at Facebook. Passionate about advancing AI-driven scientific computing, with applications in computational physics, chemistry, drug discovery, and beyond. Interested in applying quantitative methods across disciplines, including computational science, engineering, and quantitative finance.

Approved Green Card for Extraordinary Ability in Sciences (EB-1a).

Work Experience

Postdoctoral Research Fellow - Johns Hopkins University 2024 - Present

- Developing machine learning models to accelerate numerical simulations in computational chemistry
- Advancing the use of machine learning in scientific computing, particularly for modeling chemical systems.
- Investigating sampling methods for molecular dynamics, including Markov chain Monte Carlo (MCMC) techniques
- Contributing to the development of high-performance scientific software for large-scale simulations.

PhD Student, KU Leuven, Belgium 2018-2023

- Developed a micro-macro Markov chain Monte Carlo (mM-MCMC) method for multiscale molecular dynamics
- Conducted theoretical analysis, mathematical formulation, and computational implementation of the new method.
- Applied mM-MCMC on proteins and found new stable and physical conformations.

Software Engineering Intern, Facebook, London 2017

- Integrated an existing C++ physics engine into Facebook's augmented reality (AR) engine.
- Enabled the creation of more realistic visual effects, enhancing user experience.
- Project impact extends to Messenger and Instagram once deployed.

Engineering Intern, IPCOS, Leuven, Belgium 2016

- Prototyped and developed an algorithm for a mass balancing problem, reconciling estimates from a mathematical model with measured data.
- Addressed challenges with ill-conditioned data, ensuring stability and meaningful interpretation over many days.
- Implemented a solution using Regularized Recursive Least Squares with exponential memory.

Education

Master of Science: Mathematical Engineering, KU Leuven 2016-2018
Bachelor of Science: Computer Science and Electrical Engineering, KU Leuven 2013-2016

Skills & Side Projects

Technical Skills

- C++, Python, MATLAB, Javascript, Kotlin
- Cuda, Git, OpenMP, Pytorch
- HPC, Finite Element Analysis, Numerical Linear Algebra, Uncertainty Quantification
- Studying for CFA Level 1 in my free time

Open Source Projects

- **Cortisol** – A simple app to time my cortisol intake
- **PyCont** – Python package for numerical continuation and bifurcation analysis.
- **OpenMM** - Contributed to the open source molecular dynamics software