StefanDörr

PhD Biomedicine

Info

Born: 19/02/1987
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Nationality:
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Web & Git

multiscalelab.com
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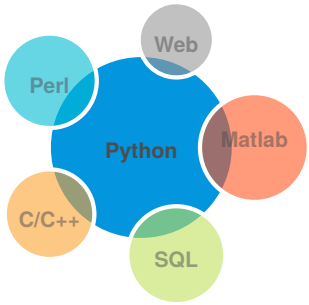
Programming



Interests

Machine learning
Deep learning
Molecular dynamics
Simulations
Markov models
Adaptive sampling

Education

2013 - 2016 **Ph.D. in Biomedicine** — Universitat Pompeu Fabra, Spain
Thesis: "Applications of machine learning in computational biology"
Awarded "Excellent (cum laude)"
Supervisor: Prof. Gianni de Fabritiis
Multiscale Lab, Barcelona, Spain

2009 - 2012 **M.Sc. in Computer Science** — Technical University Berlin, Germany
Master studies with specialization on intelligent systems and biology.
Thesis: "Sequence based retrieval of spatially contiguous structural fragments for protein structure prediction"
Supervisor: Prof. Oliver Brock
Robotics and Biology Laboratory, Berlin, Germany

2004 - 2009 **Graduate studies in Computer Science** — University of Crete, Greece
Graduate studies in computer science.
Thesis: "Two-dimensional particle systems"
Supervisor: Prof. Anthony Savidis
Foundation of Research and Technology Hellas (ICS-FORTH), Crete, Greece

2004 **High school graduation** — Heraklion, Crete, Greece
Graduated the high-school (Lyceum) in Heraklion.

Experience

2013 - 2016 **Workshop** — Acellera Ltd, Barcelona
Co-organizer of the 1st, 2nd and 3rd HTMD workshop on high-throughput molecular dynamics (workshop.htmd.org)

2014 - 2015 **Teaching** — Universitat Pompeu Fabra, Barcelona
Teaching assistant at the Master in Bioinformatics for Health Sciences at the Universitat Pompeu Fabra:
- Molecular simulations course
- Programming course using Python
- Linear algebra course

2012 - 2013 **Internship** — Acellera Ltd, Barcelona
Internship at Acellera developing methods based on Markov state models for the analysis of molecular dynamics trajectories.

05/07 2009 **Internship** — Fraunhofer Institute for Computer Graphics Research, Darmstadt
Scientific wind tunnel and liquid simulations for the automotive industry using Navier-Stokes equations. GPU accelerated soft-body simulations with CUDA.

06/09 2008 **Internship** — ICS-FORTH, Crete
Development of an XML to RDF conversion tool for the knowledge representation model CIDOC CRM (ISO21127).

Places Lived

Languages

English ★★★★★
German ★★★★★
Greek ★★★★★
Spanish ★★★☆☆

Hobbies

Dancing
Sports
Trumpet
Literature

Publications

S. Doerr, M.J. Harvey, F. Noé and G. De Fabritiis
HTMD: High-throughput molecular dynamics for molecular discovery.
J. Chem. Theory Comput., 2016, 12 (4), pp 1845–1852

S. Doerr and G. De Fabritiis
On-the-fly learning and sampling of ligand binding by high-throughput molecular simulations.
J. Chem. Theory Comput., 2014, 10 (5), pp 2064–2069

P. Bisignano, S. Doerr, M. J. Harvey, A. Favia, A. Cavalli and G. De Fabritiis
Kinetic characterization of fragment binding in AmpC β-lactamase by high-throughput molecular simulations.
J. Chem. Inf. Model., 2014, 54 (2), pp 362–366

Honors & Awards

2016 **Ph.D. award** Universitat Pompeu Fabra
Awarded excellent cum laude for the Ph.D. thesis and proposed for the PhD Extraordinary Award 2015-2016.

2010 - 2012 **DAAD scholarship** Germany
DAAD (German Academic Exchange Service) Scholarship for Masters studies in Germany.

Abbreviations

Expert (exp.)
Advanced (adv.)
Intermediate (int.)
Basic (bas.)

Software

www.htmd.org Main developer of HTMD. HTMD provides programmable framework for molecular discovery using molecular dynamics. It aims at easing access to molecular dynamics, increase reproducibility of experiments and allowing the scaling of experiments to hundreds or thousands of different simulations. Currently used by various universities and pharmaceutical companies.

Research Interests

- **Machine learning / Data mining:** Deep neural networks, dimensionality reduction, Markov models, clustering methods.
- **Computational biology:** Molecular dynamics, protein-ligand binding, protein folding, adaptive sampling methods, structure prediction, affinity prediction.
- **Software development:** Frameworks and tools for supporting biological research.

Technical skills

- **Machine learning libraries:** Scikit-learn, Keras, Theano.
- **Programming:** Python (exp.), Matlab (adv.), C++ (int.), C (int.), Java (int.), Perl (int.)
- **Web:** HTML/CSS (adv.), Django (int.), PHP (bas.), Javascript (bas.)
- **DBMS:** MySQL (int.), SQLite (bas.)

Various projects

- Computational biology
  - Protein-ligand docking using RRTs, Genetic algorithm for protein structure prediction using ROSETTA
- Web
  - Dynamic django webpage with MySQL database.
- Game development
  - ”Arkanoid” in C++, ”Monopoly” and ”Backgammon” with AI in Java, ”Multi-touch table racing game” in C#
- Robotics
  - Motion planning with RRTs, Simultaneous localization and mapping
- Mobile
  - Android application for event planning.
- Various
  - Workflow for total knee replacement in medical informatics based on new DICOM standards, Study on irresponsible research in IQ and its effects on discrimination and racism.

December, 2016

Stefan Doerr