

Rasmus Fonseca

Computer Science Ph.D.

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Experience

- 2016- Visiting Scholar at Stanford University
- Simulate GPCR conformational dynamics in Brian Kobilka's lab, Dept. of Molecular and Cellular Physiology. Secondary advisor Michael Levitt.
 - Robotics-inspired motion planning and conformational sampling of molecular complexes in Henry van den Bedem's lab, Biosciences Division, SLAC
- 2014-2015 Postdoc at Univ. Copenhagen
- High-dimensional exact and heuristic Steiner tree optimization
 - MCMC simulations of macromolecules (with Dept. of Biology)
 - Supervising bachelor projects in APL group, and course responsible 'Programming Massively Parallel Hardware', 'Python Programming' and 'Interactive Data Exploration'
- 2012-2014 Postdoc at INRIA Saclay / SLAC Stanford
- Robotics-based models for RNA molecules
 - Integrative sampling and fitting to experimental NMR data
- 2012 Research assistant at Univ. Copenhagen
- Lectures, classes and exercises in "Data Structures - Theory and Practice", "Functional Programming", and "Computer Science Theory".
- 2005-2012 Various teaching tasks at Univ. Copenhagen
- Supervision of master and bachelor projects
 - Lectures in "Computational Geometry", "Advanced Algorithms", "Algorithms and Data Structures", "Introd. to Programming", and "Protein Engineering"
 - Teaching assistant in "Object-oriented programming and design", "First year project", "Machine architecture", "Algorithms and Data structures", "Advanced Algorithms", and "Linear algebra"
- 2006-2009 Research assistant at Univ. Copenhagen
- Implementation and analysis of the chain tree data structure.
 - Implementing the educational visual micro architecture simulator KredsDesign, for the Machine Architecture course.

Education

- 2009 to 2012 Ph.D. student at Univ. Copenhagen, Department of Computer Science.
- PhD project supervised by Pawel Winter: Reducing the Search Space in Protein Structure Prediction.
 - Stay at University of California Santa Cruz, USA, 2010-2011. Collaboration with Professor Kevin Karplus
- 2005-2009 Grad studies (Cand.Scient.) Computer Science, Univ. Copenhagen
- Master thesis supervised by Pawel Winter: "Ab Initio Protein Structure Prediction using Bezier Curve Representation". Grade 12 (A)
 - Courses: "Neural Networks", "Advanced Algorithms", "Intro to Optimization", "Efficient AI programming", "Comp. Geometry", "Algorithms in Bioinformatics".
- 2001-2005 Undergraduate studies (Cand.Bach.) Univ. Copenhagen
- Bach.Scient. Physics major, computer science minor
 - Courses: Basic courses in physics and computer science plus: Quantum physics, Statistical physics, Computer physics, Optics, Human computer interaction, and Introduction to graphics.

Skills

At least two year experience using each of the following languages/frameworks

- C/C++, CUDA, lapack/Intel MKL
- Python, numpy, pandas, scikit-learn, pyplot, seaborn
- Java, Java3D, Swing, JavaFX
- JavaScript, D3.js, Three.js
- Bash, data management (sed/grep/etc), make, ssh/rsync,

Contributed to the following software projects

- ProGAL, an open-source Java-library containing geometric algorithms and data structures used for protein representations and analysis (Delaunay tessellations, object collisions, principal components analysis).
- Markov Chain Monte Carlo, Inverse Kinematic robotics-inspired, and chain-tree bounding volume hierarchy for conformational changes and free-energy estimates in molecular systems.
- Participated in the 11th DIMACS challenge with my code to solve the Euclidean Steiner Minimal Tree problem.
- Data visualization such as matrix bubble plot and flare plots for dynamic network visualization

See specific projects at <https://rasmusfonseca.github.io>.

Teaching:

- Eight years of experience teaching, both as a classroom TA and lecturer
- Computer architecture, linear algebra, advanced algorithms, functional programming, parallel programming, machine learning, and interactive data visualization.

Awards and funding

Novo nordisk foundation visiting scholar fellowship at Stanford Bio-X. Four year research grant to visit Brian Kobilka's lab at Stanford investigating GPCR activation mechanisms using computational methods, 2016-2018.

FIRST / Dept. of Computer Science / Faculty of Science PhD fellowship. Jointly funded three year PhD fellowship to investigate "Reducing the Search Space in Protein Structure Prediction", 2009-2011

Danish society of Computer Science - Best master thesis award 2009

Selected publications

Characterizing RNA ensembles from NMR data with kinematic models

R Fonseca, DV Pachov, J Bernauer, H Van den Bedem
Nucleic acids research 42 (15), 9562-9572

Collision-Free Poisson Motion Planning in Ultra High-Dimensional Molecular Conformation Spaces

R Fonseca, D Budday, H Bedem
arXiv preprint arXiv:1607.07483

Coupled motions in β 2AR: Gas conformational ensembles

DV Pachov, R Fonseca, D Arnol, J Bernauer, H van den Bedem
Journal of chemical theory and computation 12 (3), 946-956

See a full list at: <http://orcid.org/0000-0002-8322-4880>