

Oleg Trott, Ph.D.

Staff Scientist

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Summary

A Columbia-educated Ph.D. with a solid background in physics and applied math, extensive programming experience in C++ and other languages and a proven track record of successfully applying mathematical methods, numerical analysis and machine learning to complex real-world problems

Education

Columbia University

New York, NY

- Ph.D. 2004
Thesis topic: Protein dynamics and its prediction using machine learning

Moscow Institute of Physics and Technology (PhysTech)

Moscow, Russia

- B.Sc. 1997
Physics and Applied Mathematics specialization

Personal Information

- U.S. Permanent Resident

Technical Skills

- **Computer Languages:** C++ (including STL and some Boost libraries), Python, OCaml, MATLAB, Lisp, Prolog, Bourne Shell, \LaTeX , PostScript
- **Operating Systems:** Windows, Linux, OS X, FreeBSD, IRIX
- **Mathematical methods:** linear algebra, matrix theory, differential equations, perturbation theory and many others
- **Numerical analysis:** numerical optimization, eigensystem problems, numerical solution of systems of differential equations, global optimization
- **Data analysis:** statistical analysis, machine learning

Professional Experience

- **Staff Scientist, The Scripps Research Institute (2009-2011)**
- **Research Associate, The Scripps Research Institute (2006-2009)**

At Scripps, I worked on software that computationally predicts the interaction of drug molecules with their targets (proteins), which is, in a sense, a machine learning and global optimization problem. I designed and fully implemented in C++ a new program of this kind, AutoDock Vina (vina.scripps.edu). My program achieves a 10- to 100-fold speed-up compared to the analogous software previously developed by my employer (AutoDock 4), while also significantly improving the accuracy of the predictions. Further speed-up is achieved via parallelism on multi-core machines.

- **Research Assistant, Columbia University (1997-2004)**

At Columbia, I performed mathematical analyses of NMR methods used to study biological systems at atomic resolution, thereby advancing their state of the art. This work drew on several mathematical subjects, including linear algebra, differential equations and the perturbation theory. In a separate project, I designed and implemented in C++ a supervised machine learning system used to predict the flexibility of proteins from their 3D structures.

Publications

- O. Trott, A. J. Olson, AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization and multithreading, *Journal of Computational Chemistry* 31 (2010) 455-461
- O. Trott, K. Siggers, B. Rost, A. G. Palmer, Protein conformational flexibility prediction using machine learning, *Journal of Magnetic Resonance* 192 (2008) 37-47
- O. Trott, Ph.D. Thesis: Protein dynamics and its prediction using machine learning, *Columbia University* (2004)
- O. Trott, A. G. Palmer, Theoretical study of $R_{1\rho}$ rotating-frame and R_2 free-precession relaxation in the presence of n -site chemical exchange, *Journal of Magnetic Resonance* 170 (2004) 104-112
- O. Trott, D. Abergel, A. G. Palmer, An average-magnetization analysis of $R_{1\rho}$ relaxation outside of the fast-exchange limit, *Molecular Physics* 101-6 (2003) 753-763
- L. Vugmeyster, O. Trott, C. J. McKnight, D. P. Raleigh, A. G. Palmer, Temperature-dependent dynamics of the villin headpiece helical subdomain, an unusually small thermostable protein, *Journal of Molecular Biology* 320 (2002) 841-854
- O. Trott, A. G. Palmer, $R_{1\rho}$ relaxation outside of the fast-exchange limit, *Journal of Magnetic Resonance* 154 (2002) 157-160