

# 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 applying mathematical methods, numerical analysis and machine learning to complex real-world problems

## Education

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| <b>Columbia University</b>   | New York, NY   |
| • Ph.D. 2004   |                |
| Thesis topic: Protein dynamics and its prediction using machine learning |                |
| <b>Moscow Institute of Physics and Technology (PhysTech)</b>             | Moscow, Russia |
| • B.Sc. 1997   |                |
| Physics and Applied Mathematics specialization                           |                |

## Professional Interests

- Machine learning, data mining, artificial intelligence and numerical methods, as well as their applications to life sciences

## Technical Skills

- **Computer Languages:** C++, Python, O'Caml, MATLAB, Lisp, Prolog, Bourne Shell, L<sup>A</sup>T<sub>E</sub>X, PostScript
- **Operating Systems:** Windows, Linux, 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
- **Data analysis:** statistical analysis, supervised machine learning, artificial neural networks
- **Bioinformatics:** molecular docking, protein structure analysis, secondary structure determination, flexibility prediction

## Research Experience

### Doctoral Research (1997-2004)

Columbia University

Integrated Program in Cellular, Molecular and Biophysical Studies

Research Advisor: Prof. Arthur G. Palmer III

Most of the results of my graduate research are described in my doctoral dissertation available at [digitalcommons.libraries.columbia.edu/dissertations/AAI3129038/](http://digitalcommons.libraries.columbia.edu/dissertations/AAI3129038/). My work focused mainly on these topics:

- *Theoretical study of  $R_{1\rho}$  relaxation in the presence of chemical exchange:* In NMR,  $R_{1\rho}$  relaxation refers to the evolution of the nuclear spin magnetization in the presence of a weak radio frequency field.  $R_{1\rho}$  relaxation is affected by the dynamical changes in molecular structure. While the underlying principles have been known for decades, the interplay of  $R_{1\rho}$  relaxation and protein dynamics is complex, and analytical results existed only for very restricted special cases. Our mathematical analysis of  $R_{1\rho}$  spin relaxation gave us both general theoretical results and insights into using  $R_{1\rho}$  relaxation to study microsecond to millisecond time scale protein dynamics. This work involved both mathematical analysis and numerical simulations, drawing from various fields, such as linear algebra, Markov processes and perturbation theory.
- *Prediction of conformational flexibility of proteins using artificial neural networks:* Traditionally, Molecular Dynamics simulations are used to predict the flexibility of macromolecules. While such simulations can provide vast amounts of data, they are very computationally expensive and have limited accuracy. We applied artificial neural networks to perform a "learning from examples" based on existing NMR data of nanosecond time scale protein dynamics. The results are used to make predictions about structures of unknown flexibility. This project involved processing Protein Data Bank data files, numerical optimizations, simulated annealing, various supervised machine learning methods and statistical analysis.

### Postdoctoral Research (2006-2009)

The Scripps Research Institute

Molecular Graphics Lab

During my postdoctoral work, I designed and implemented a new molecular docking program, AutoDock Vina ([vina.scripps.edu](http://vina.scripps.edu)), that achieves a 10- to 100-fold speed-up compared to the molecular docking software previously developed in the lab (AutoDock 4), while also significantly improving the accuracy of the predictions. Further speed-up is achieved from parallelism, by using multithreading on multi-core machines.

## 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