

Academic Seminar on Optimal Protein Structure Alignment Using Maximum Cliques

Jointly Organised by

**The Logistics Institute – Asia Pacific
&
Industrial & Systems Engineering Department
Faculty of Engineering, NUS**

Wednesday, 10 March 2004 3:30pm
Seminar Room EA-06-02
Faculty of Engineering
National University of Singapore
([Location Map](#))

• About the Speaker •

Dr. Joel Sokol

Assistant Professor
Georgia Institute of Technology
<http://www.isye.gatech.edu/people/profile.php?id=1324>



Joel Sokol is an assistant professor in Industrial and Systems Engineering at the Georgia Institute of Technology. He received a Ph.D. in operations research from the Massachusetts Institute of Technology in 1999. His bachelor's degrees, including a B.S. in applied sciences in engineering and a B.A. in mathematics and computer science are from Rutgers University, where he graduated first in his class. Dr. Sokol's research interests include networks, linear programming, inverse optimization, and combinatorial optimization, as well as the application of operations research techniques to logistics, transportation, and network design problems. He is also interested in applications in biology, social logistics, and sports modeling.

• About the Seminar •

In biology, the protein structure alignment problem answers the question of how similar two proteins are. Proteins with strong physical similarities in their tertiary (folded) structure often have similar functions, so understanding physical similarity could be a key to developing protein-based medical treatments. Currently, the best model for protein structure alignment is the maximum contact map overlap (CMO) model. The CMO model of protein structure alignment is NP-hard and can be cast as a maximum clique problem on an appropriately defined graph. We prove and exploit properties of these protein-based maximum clique problems to develop specialized preprocessing techniques, and show how they can be used to more quickly solve contact map overlap instances to optimality.

• Program at a Glance •

- 3.30 pm : Brief Introduction by Prof Huang Huei Chuen
 Industrial & Systems Engineering Department
 Faculty of Engineering, National University of Singapore
- 3.35pm to 4.30 pm : Lecture by Dr. Joel Sokol
 (Including a Question & Answer Session)

• Other Information •

Admission is free. Seats are limited to the first 80 participants on a first come first serve basis. This invitation extends to

- NUS Faculty Members, Research Staff and Students (specifically, from Faculty of Engineering, Faculty of Science - Maths and Statistics Departments, School of Business - Decision Science Department, and School of Computing)
- All members of TLI-Asia Pacific Supporting Government Agencies and Operational Research Society of Singapore
- Members of the Logistics Industry & Professions
- TLI-Asia Pacific Faculty Members, Research Staff and Dual MSc Students