

Yiannis N. Kaznessis

Associate Professor

Department of Chemical Engineering and Materials Science, and Digital Technology Center,
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Professor Kaznessis' research interests focus on computer modeling of biological matter, synthetic biology and on statistical mechanical modeling of biomolecular recognition phenomena. Professor Kaznessis teaches undergraduate "Chemical Engineering Thermodynamics", undergraduate "Process Dynamics and Control" and the graduate course "Statistical Thermodynamics and Kinetics". Professor Kaznessis is also the Director of the University of Minnesota Summer Bioinformatics Institute.

Education

- Diploma, Chemical Engineering, Aristotle University of Thessaloniki, Greece, 1994.
- Ph.D., Chemical Engineering, University of Notre Dame, 2000.
- Postdoctoral Fellowship, University of Michigan and Pfizer Global Research and Development, 08/99-08/01

Appointments

ASSOCIATE PROFESSOR, 08/01/07-

Department of Chemical Engineering and Materials Science, University of Minnesota
Digital Technology Center, University of Minnesota

ASSISTANT PROFESSOR, 08/23/01-07/31/07

Department of Chemical Engineering and Materials Science, University of Minnesota
Digital Technology Center, University of Minnesota

DIRECTOR, 01/01/03-present

University of Minnesota Summer Bioinformatics Institute

POSTDOCTORAL FELLOW, 08/99-08/01

Biomolecular Structure and Drug Design, Pfizer Global Research and Development.
Department of Chemical Engineering, University of Michigan.

RESEARCH ASSISTANT, 09/94-08/99

Department of Chemical Engineering, University of Notre Dame, Ph.D. (2000).

PROJECT MANAGER ASSISTANT, 12/93-08/94

Euroconsultants S.A., Thessaloniki, Greece.

RESEARCH ASSISTANT, 01/91-05/92

Chemical Process Engineering Research Institute, Thessaloniki, Greece.

Honors and Awards

- 2007 NSF CAREER
 - 2006 Fellow, Minnesota Supercomputing Institute
 - 2004 3M non-Tenured Faculty Award
 - 2003 IBM Young Faculty Award
 - 2003 Young Investigator Petroleum Research Fund Award
 - 2000 Postdoctoral Fellowship, University of Michigan/Pfizer GRD
 - 2000 SGI Computational Science and Visualization Award, University of Notre Dame
 - 1994 Fulbright Award
 - 1994 Technical Chamber of Greece Honor Award (1st in senior class)
 - 1991-1993, Greek National Fellowship Foundation Awards (IKY)
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Research Publications

1. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, "Molecular Dynamics Simulations of Polar Polymer Brushes", *Macromolecules*, Vol. 31, p. 3116, 1998.
 2. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, "A Molecular Dynamics Study of Macromolecules in Good Solvents. Comparison with Dielectric Spectroscopy Experiments", *Journal of Chemical Physics*, Vol. 109, p. 5078, 1998.
 3. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, "Dielectric Relaxation of Dipole-Inverted Macromolecules Using Computer Simulations", *Macromolecules*, Vol. 32, p. 6679, 1999.
 4. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, "Concentration and Size Dependence of Dielectric Strength and Dielectric Relaxation of Flexible Polymers in Dilute and Semidilute Solutions of a Theta Solvent", *Macromolecules*, Vol. 32, p. 1284, 1999.
 5. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, "Dielectric Relaxation of Concentrated Polymer Solutions via Molecular Dynamics Simulations", *Journal of Chemical Physics*, Vol. 111, p. 1325, 1999.
 6. Y. N. Kaznessis, L. Narashimhan, M. E. Snow, "Binding Free Energy Calculations for Benzamide-Trypsin Complexes", *Proceedings of Foundations of Molecular Modeling and Simulation Conference, AIChE Symposium Series*, p. 283, 2000.
 7. Y. N. Kaznessis, M. E. Snow, C. J. Blankley, "Prediction of Blood-Brain Partitioning Using Monte-Carlo Simulations of Molecules in Water", *Journal of Computer-Aided Molecular Design*, Vol. 15, p. 697, 2001.
 8. Y. N. Kaznessis, S. Kim, R. G. Larson, "Simulations of Zwitterionic and Anionic Phospholipid Monolayers", *Biophysical Journal*, Vol. 82, p. 1731-42, 2002.
 9. Y. N. Kaznessis, S. Kim, R. G. Larson, "Specific Mode of Interaction Between Components of Model Pulmonary Surfactants Using Computer Simulations", *Journal of Molecular Biology*, Vol. 322, p. 569-582, 2002.
 10. L.M. Gordon, P.W. Mobley, W. Lee, S. Eskandari, Y. Kaznessis, M.A. Sherman, A.J. Waring, "Conformational mapping of the N-terminal peptide of HIV-1 GP41 in lipid detergent and aqueous environments using ^{13}C -enhanced Fourier transform infrared spectroscopy" *Protein Science*, Vol. 13, p. 1012-30, 2004.
 11. H. Wei, Y. Kaznessis, "Inferring gene regulatory relationships by combining target-target pattern recognition and regulator-specific motif examination" *Biotechnology and Bioengineering*, Vol. 89(1), p. 52-77, 2005.
 12. N. Ostberg, H. Khandelia, Y. Kaznessis, "Protegrin structure activity relationships: Using homology models of synthetic sequences to determine structural characteristics important for activity" *Peptides*, Vol. 26(2), p. 297-306, 2005.
 13. A. Langham, Y. Kaznessis, "Molecular dynamics simulations of the N-terminus of HIV GP-41 fusion peptide in SDS micelles" *Journal of Peptide Science*, Vol. 14(2), p. 316-328, 2005.
 14. S. Vicatos, V.B. Reddy, Y. Kaznessis, "Prediction of distant residue contacts with the use of evolutionary information" *Proteins, Bioinformatics, Structure and Genetics*, Vol. 58(4): 935-49, 2005.
 15. H. Salis, Y. Kaznessis, "Accurate Hybrid Stochastic Simulation of a System of Coupled Chemical or Biochemical Reactions", *Journal of Chemical Physics*, Vol. 122, p. 054103 1-13, 2005.
 16. H. Salis, Y. Kaznessis, "Numerical simulation of stochastic gene circuits" *Computers & Chemical Engineering*, Vol 29(3), p. 577-588, 2005.
 17. Y. Duan, V. Reddy, Y. Kaznessis, "Physicochemical and residue conservation calculations to improve the ranking of protein-protein docking solutions" *Protein Science*, Vol. 14(2), p.316-328, 2005.
 18. H. Khandelia, Y. Kaznessis, "Molecular dynamics simulations of the helical antimicrobial peptide ovispirin-1 in zwitterionic dodecylphosphocholine micelles: Insights into host-cell toxicity" *Journal of Physical Chemistry B*, Vol. 109(26) p. 12990 – 12996, 2005.
 19. V. Reddy, Y. Kaznessis, "Quantitative analysis of interfacial amino acid conservation in protein-protein hetero complexes" *Journal of Bioinformatics and Computational Biology*, Vol. 3(5), p.1137-50, 2005.
 20. H. Khandelia, Y. Kaznessis, "Molecular dynamics simulations of helical antimicrobial peptides in SDS micelles: What do point mutations achieve?" *Peptides*, Vol. 26(11), p. 2037-2049, 2005.
 21. H. Salis, Y. Kaznessis "An equation-free probabilistic steady state approximation: Dynamic application to the stochastic simulation of biochemical reaction networks", *Journal of Chemical Physics*, Vol. 123(21), p. 214106, 2005
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22. A. Langham, H. Khandelia, Y. Kaznessis, "How can protegrin-1 be both a potent antimicrobial and harmfully toxic?: Molecular dynamics simulations of a beta-sheet antimicrobial peptide in micelles" *Biopolymers: Peptide Science*, Vol. 84 (2), p.219-231, 2006.
 23. L. Tuttle, H. Salis, J. Tomshine, Y. Kaznessis, "Model-Driven Design Principles of Gene Networks: the Oscillator", *Biophysical Journal*, Vol. 89(6), p. 3873-83, 2005
 24. Y. Kaznessis, "Multi-Scale Models for Gene Network Engineering", *Chemical Engineering Science*, Vol. 61(3), p. 940-953, 2006.
 25. Y. Kaznessis, "A review of methods in computational prediction of blood-brain partitioning" *Current Medicinal Chemistry, Central Nervous System Agents*, Vol. 5, (3), p.185-191, 2005.
 26. H. Salis, V. Sotiropoulos, Y. Kaznessis "Multiscale Hy3S: Hybrid Stochastic Simulations for Supercomputers", *BMC Bioinformatics*, (highly accessed), Vol. 7:93, 2006.
 27. H. Khandelia, Y. Kaznessis, "Molecular Dynamics Investigation of the Influence of Anionic and Zwitterionic Interfaces on Antimicrobial Peptides' Structure: Implications on Peptide Toxicity and Activity" *Peptides*, Vol. 27(6), p.1192-1200, 2006.
 28. Y. Duan, B. Reddy, Y. Kaznessis "Residue conservation information for generating near-native structures in protein-protein docking" *Journal of Bioinformatics and Computational Biology*, 4:793-806, 2006.
 29. H. Khandelia, A. Langham, Y. Kaznessis, "Driving engineering of novel antimicrobial peptides from simulations of peptide-micelle interactions", *BBA, Biomembranes*, 1758(9):1224-34, 2006.
 30. W. Wang, C. Mulakala, S.C. Ward, G. Jung, H. Luong, D. Pham, A.J. Waring, Y. Kaznessis, W. Lu, K.A. Bradley, R.I. Lehrer. "Retrocyclins kill bacilli and germinating spores of *Bacillus anthracis* and inactivate anthrax lethal toxin." *Journal of Biological Chemistry*, 281(43):32755-64, 2006.
 31. J. Tomshine, Y. Kaznessis, "Optimization of a stochastically-simulated gene network model via simulated annealing", *Biophys J.* 91(9):3196-205, 2006.
 32. A. Langham, Y. Kaznessis "Effects of mutations on the C-terminus of protegrin-1: a molecular dynamics simulation study", *Molecular Simulation*, 32(3-4):193-201, 2006.
 33. H. Salis, Y. Kaznessis, "Computer-aided design of modular protein devices: Boolean AND gene activation." *Phys Biol.* 3(4):295-310, 2006.
 34. V. Sotiropoulos, Y. Kaznessis, "Synthetic tetracycline-inducible regulatory networks: computer-aided design of dynamic phenotypes" *BMC Systems Biology*, 1:7, 2007
 35. C. Mulakala, J.D. Lambris, Y. Kaznessis, "A simple, yet highly accurate, QSAR model captures the complement inhibitory activity of compstatin", *Bioorg Med Chem.* 15(4):1638-44, 2007.
 36. H. Khandelia, Y. Kaznessis, "Structure of the Antimicrobial β -hairpin Peptide Protegrin-1 in a DLPC Lipid Bilayer Investigated by Molecular Dynamics Simulation", *BBA Biomembranes*, 1768(3):509-20, 2007.
 37. H. Khandelia, Y. Kaznessis, "Cation- π Interactions Stabilize the Structure of the Antimicrobial Peptide Indolicidin near Membranes: Molecular Dynamics Simulations", *J. Phys. Chem. B*, 111(1):242-250, 2007
 38. D. Bolintineanu, A. Langham, T.H. Davis, Y. Kaznessis, "Molecular dynamics simulations of three protegrin-type anti-microbial peptides: interplay between charges at the termini, β -sheet structure and amphiphilic interactions", *Molecular Simulation*, 2007, 33, 809 – 819.
 39. A. Langham, A.J. Waring, Y. Kaznessis, "Comparison of interactions between β -hairpin decapeptides and SDS/DPC micelles from experimental and simulation data", *BMC Biochemistry*, 2007 Jul 16;8(1):11.
 40. S. Vicatos, Y. Kaznessis, "Separating true positive predicted residue contacts from false positive ones in mainly alpha proteins, using constrained Metropolis MC simulations." *Proteins*, 2008 Feb 1;70(2):539-52
 41. V. Sotiropoulos, Y.N. Kaznessis "An Adaptive Time Step Scheme for a System of SDE's with Multiple Multiplicative Noise. Chemical Langevin Equation, a proof of concept", *J. Chem. Phys.* 2008 Jan 7;128(1):014103.
 42. Reddy BV, Kaznessis YN. "Use of secondary structural information and C alpha-C alpha distance restraints to model protein structures with MODELLER." *J Biosci.* 2007 Aug;32(5):929-36.
 43. Kaznessis YN. "Models for synthetic biology." *BMC Syst Biol.* 2007 Nov 6;1(1):47
 44. A. Langham, H. Khandelia, B. Schuster, A. Waring, R. Lehrer, Y. Kaznessis "Correlation between simulated physicochemical properties and hemolysis of protegrin-like antimicrobial peptides: Predicting experimental toxicity" *Peptides*, 2008, 29(7): 1085-1093.
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45. A. Hill, J. Tomshine, E. Wedding, V. Sotiropoulos, Y. Kaznessis, "SynBioSS: the Synthetic Biology Modeling Suite", *Bioinformatics* 2008, 24(21):2551-3.
46. Chatterjee A, Kaznessis YN, Hu WS. Tweaking biological switches through a better understanding of bistability behavior. *Curr Opin Biotechnol.* 2008 Oct;19(5):475-81.
47. Chiu TL, Mulakala C, Lambris JD, Kaznessis YN., Development of a new pharmacophore model that discriminates active compstatin analogs. *Chem Biol Drug Des.* 2008 Oct;72(4):249-56.
48. Langham A., Sayyed-Ahmad A, Kaznessis YN, "On the nature of antimicrobial activity: a model for Protegrin-1 pores", *JACS*, 2008, 130(13): 4338-4346
49. V. Sotiropoulos, P. Daoutidis, YN Kaznessis, "Model Reduction of Multiscale Chemical Langevin Equations: A Numerical Case Study", *IEEE Transactions in Computational Biology and Bioinformatics*, 2009, in press.
50. D. Bolintineanu, HT. Davis, YN. Kaznessis, "Poisson-Nernst-Planck models of nonequilibrium ion electrodiffusion through a protegrin transmembrane pore", *PLoS Computational Biology*, 2009, in press

Invited and Conference Presentations since 2005

- Y. Kaznessis, "Multiscale Models for Synthetic Biology", *Advances in Synthetic Biology*, April 2009, London, England, invited presentation
 - Y. Kaznessis, "Computer-Aided Designs of Antimicrobial Peptides", *Gordon Conference on Antimicrobial Peptides*, March 2009, CA
 - Y. Kaznessis, "Multiscale Models for Synthetic Biology", *Rensselaer Polytechnic Institute*, January 2009, invited presentation.
 - Y. Kaznessis, "Multiscale Models for Synthetic Biology", *Princeton University*, December 2008, invited presentation.
 - Y. Kaznessis and 10 Bioinformatics Summer Institute undergraduates, "Synthetic Bio-Logical AND gates", *iGEM 2008*, November 2008, Boston, MA
 - J Tomshine, Y. Kaznessis, "Bio-logical AND gates", *Synthetic Biology 4.0*, October, 2008, Hong Kong, China
 - Y. Kaznessis, "Multiscale Models for Synthetic Biology", *International Conference of Systems Biology*, August 2008, Gothenburg, Sweden, invited presentation.
 - Y. Kaznessis, "Multiscale Models for Synthetic Biology", *WORDOCOM 08*, July 2008, Las Vegas NV, invited presentation.
 - Y. Kaznessis, "Multiscale Models for Synthetic Biology", *Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean Countries*, May 2008, Cetraro, Italy, invited presentation.
 - Y. Kaznessis, "Synthetic Bio-logical AND gates", *Synthetic Biology 3.0*, Zurich, Switzerland, July 2007
 - Y. Kaznessis, "Synthetic Bio-logical AND gates", *Pathways, Networks and Systems Biology*, Porto Heli, Greece, July 2007.
 - Y. Kaznessis, "Model-Driven Synthetic Bioengineering", *PPEPPED 2007*, Crete, Greece, June 2007.
 - A. Langham, "Computer-Driven Antimicrobial Peptide, Engineering", *2007 Biophysical Meeting*, Baltimore, March 2007.
 - Howard Salis, Yiannis N. Kaznessis, "Bifurcation Analysis of Stochastic Gene Networks", *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
 - Vassilios Sotiropoulos, Marie-Nathalie Contou-Carrere, Prodromos Daoutidis, Yiannis N. Kaznessis, "Reduction of Multi-Scale Systems of Chemical Langevin Equations", *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
 - Himanshu Khandelia, Yiannis N. Kaznessis, "Molecular Dynamics Simulations to Guide the Design of Peptide Antibiotics", *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
 - Howard Salis, Yiannis N. Kaznessis, "Computer Aided Design of Modular Protein Devices: Logical "and" Gene Activation", *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
 - Abdallah Sayyed-Ahmad, Yiannis Kaznessis, "Relative Binding Free Energy Calculations of Antimicrobial Peptides in Sds/Dpc Micelles Using Molecular Dynamics/Continuum Methods", *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2006.
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- Allison Langham, Yiannis N. Kaznessis, "The Design of New Protegrin-like Antimicrobial Peptides: a Molecular Dynamics Study", American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
 - Jonathan R. Tomshine, Yiannis N. Kaznessis, "Optimization of Stochastically-Simulated Gene Network Models", American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
 - Spyridon Vicatos, Yiannis Kaznessis, "Separating True Positive Residue Contacts from False Positive Ones in Proteins, Using Constrained Metropolis Monte Carlo Simulations", American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
 - Vassilios Sotiropoulos, Yiannis N. Kaznessis, "In Silico Design of Synthetic Tetracycline-Inducible Regulatory Gene Networks", American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
 - Y. Kaznessis, "The New Mathematics of Biological Engineering", presentation, International Conference in Bioengineering and Nanotechnology, Santa Barbara, CA, September, 2006.
 - H. Salis, Y. Kaznessis, "Multi-Scale Models for Gene Network Engineering", Raleigh, NC, August, 2006
 - Y. Kaznessis, "The New Mathematics of Biological Engineering", invited presentation, Iowa State University, April 2006.
 - A. Langham, Y. Kaznessis, "Simulations of Protegrin-1, a potent antimicrobial peptide", Biophysical Society Meeting, San Francisco, CA, 2006
 - H. Khandelia, Y. Kaznessis "Molecular Dynamics Simulations of Antimicrobial Peptides" Platform presentation, American Chemical Society, Atlanta, GA, 2006
 - A. Langham, Y. Kaznessis, "Simulations of Protegrin-1, a potent antimicrobial peptide", Biophysical Society Meeting, San Francisco, CA, 2006
 - H. Salis, Y. Kaznessis, "Model-Driven Designs of Gene Regulatory Networks", Platform presentation, Biophysical Society Meeting, San Francisco, CA, 2006
 - H. Khandelia, Y. Kaznessis "Molecular Dynamics Simulations of Antimicrobial Peptides" Platform presentation, Biophysical Society Meeting, San Francisco, CA, 2006
 - Y. Kaznessis, "Multiscale Models for Gene Network Engineering", invited presentation, National Technical University, Athens, Greece, January 2006
 - Marie-Nathalie Contou-Carrere, P. Daoutidis, Y. Kaznessis "Model Reduction of Multi Scale Chemical Langevin Equations", 2005 Annual AIChE Meeting, Cincinnati, OH, November 2005
 - H. Salis, Y. Kaznessis, "Equation-Free Probabilistic Steady State Approximation: Dynamic Application to the Stochastic Simulation of Chemically Reacting Systems", 2005 Annual AIChE Meeting, Cincinnati, OH, November 2005
 - Y. Kaznessis, V. Sotiropoulos, "Model-Driven Engineering of Regulatable Gene Networks", 2005 Annual AIChE Meeting, Cincinnati, OH, November 2005.
 - H. Khandelia, Y. Kaznessis, "Antimicrobial Peptides and Implications on Peptide Toxicity and Activity: a Molecular Dynamics Simulation Investigation", 2005 Annual AIChE Meeting, Cincinnati, OH, November 2005.
 - Y. Kaznessis, "Computer-Aided Design of Gene Regulatory Networks: Trends and Prospects", Invited presentation at the International Symposium on Biotechnology Trends, Past and Future, at the University of Minnesota Biotechnology Institute, Minneapolis, October, 2005
 - Y. Kaznessis, "Modeling and Design of Antimicrobial Peptides", invited presentation, UCLA, August 2005
 - H. Salis, Y. Kaznessis, "Computational Design of Oscillating Gene Regulatory Networks", Foundations of Systems Biology in Engineering, Santa Barbara, August 2005.
 - H. Salis, Y. Kaznessis, "Computational Design of Oscillating Gene Regulatory Networks" XIV Bioengineering Conference, Harrison Springs, CA, July 2005
 - Y. Kaznessis, "Computational Modeling and Design of Proteins" invited presentation, Beckman-Coulter, July 2005.
 - H. Salis, Y. Kaznessis, "De Novo Design of Gene Regulatory Networks" Workshop in High-Performance Computational Models for Molecular Recognition and Biosensing" Santa Barbara, July 2005.
 - H. Khandelia, Y. Kaznessis "Effect of Mutations on the Toxicity of Small Helical Antimicrobial Peptides: Insights from Molecular Dynamics Simulations in Zwitterionic Micelles", Protein Society Annual Meeting, Boston, MA, July 2005
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- A. Langham, Y. Kaznessis “The Effects of Mutations on Toxicity on beta-hairpin Antimicrobial Peptides: Simulations in SDS and DPC Micelles” Protein Society Annual Meeting, Boston, MA, July 2005
- Y. Kaznessis, “Multi-scale Models for Gene Network Engineering”, 2005 Midwest Thermodynamics and Statistical Mechanics Conference, West Lafayette, IN, May 2005.
- Y. Kaznessis, “Model-Driven Designs of Gene Regulatory Networks”, invited presentation, March 2005, Purdue University
- Y. Kaznessis, “Identification of Protein-Protein Interaction Sites”, invited presentation, February 2005, University of Pennsylvania.
- H. Khandelia, Y. Kaznessis, “Molecular Dynamics Simulations of Helical Antimicrobial Peptides in SDS micelles: What do Point Mutations Achieve?” Platform presentation, 2005 Biophysical Society Meeting, Long Beach, CA.
- A. Langham, Y. Kaznessis, “What Makes Protegrin Analogues Antimicrobial?”, poster presentation, 2005 Biophysical Society Meeting, Long Beach, CA.
- H. Khandelia, Y. Kaznessis, “Adding Dynamics in Structural Bioinformatics: the Case of Antimicrobial Peptides”. Presentation at the International Conference of Bioinformatics, January 2005, Singapore

Membership

American Institute of Chemical Engineers, American Chemical Society

Professional Activities - Service

- Director, Area 15, AIChE, 2008-
- Chair of programming, Area 10d, AIChE, 2009
- Chair, Faculty Search Committee, CEMS 2009
- Director, University of Minnesota Bioinformatics Summer Institute
- Editorial Board, BMC Systems Biology
- Chair, Steering Committee, Unisys/Minnesota Supercomputing Institute Alliance
- Fellow, Minnesota Supercomputing Institute
- Member, Internal Advisory Committee, Minnesota Supercomputing Institute
- Member, NSF Partnership for Advanced Computational Infrastructure Committee
- Member, NIH Review Panel, NIH Pathway to Independence Award
- Member, Advisory Committee, University of Minnesota Digital Technology Center
- Member, Steering Committee, University of Minnesota Computational Genetic Laboratory
- **Past service:** Member, Graduate Admissions Committee, CEMS
- Vice Chair, Computational Genomics, 2006 AIChE Annual Meeting
- Member, Organizing Committee, 2007 Bioengineering Conference; Member, Organizing Committee, 2005 Foundations of Systems Biology and Engineering Conference; Vice Chair, Biomedical Applications of Systems Biology Session, 2005 AIChE Annual Meeting; Member, Faculty Recruiting Committee, Department of Computer Science and Engineering; Member, Chemical Engineering Curriculum Committee (2003), CEMS; Vice Chair, Bioinformatics Topical Conference, 2001 AIChE Annual Meeting; Chair, Group T3, Bioinformatics, 2002 AIChE Annual Meeting; Member, NSF SBIR 2004 panel; Member, NSF Emerging Models and Technologies (EMT) 2004 and 2005 panels
- Reviewer of manuscripts in: Biophysical Journal, Biological Macromolecules, Biochimica & Biophysica Acta, Bioorganic and Medicinal Chemistry, BMC Bioinformatics, Biotechnology and Bioengineering, Computers and Chemical Engineering, Journal of Biotechnology, Journal of Physical Chemistry, Journal of Chemical Physics, Langmuir, Molecular Simulation, Physical Biology, Proteins, JACS, Biochemistry

Research Group

Graduate students: Katherine Volzing, Apostolos Vagias, Kostas Billiouris, Ben Swiniarski, Jonathan Tomshine, Vassilis Sotiropoulos, Dan Bolintineanu, John Barrett, Nagendra Singh, Anushree Chatterjee

Postdoctoral Fellows: Abdallah Sayyed-Ahmad, Ting-Lan Chiu, Chandrika Mulakala, Poonam Shrivastava, Victor Vivcharuk, Emilia Wu

Past Group Members

Allison Langham (Ph.D. 2008) now at the Pentagon.

Spyros Vicatos (Ph.D. 2007) now postdoctoral fellow at the University of Southern California.

Himanshu Khandelia (Ph.D. 2006) now postdoctoral fellow at the University of Southern Denmark

Howard Salis (Ph.D. 2007) now postdoctoral fellow at the University of California, San Francisco

Nathan Ostberg (M.Sc), Lisa Tuttle (BSI and M.Sc.)

Yuhua Duan (postdoctoral fellow, now at DOE National Energy Technology Laboratory)

Boojala Reddy (research associate, now assistant professor at CUNY)

Hairong Wei (postdoctoral fellow, now Assistant Professor at Michigan Tech)

Kavita Iyer (postdoctoral fellow, now at Merck).

Anthony Hill (postdoctoral fellow, now at St. Jude's)

Another four chemical engineering undergraduate students have worked in our group, along with seventeen Bioinformatics Summer Institute interns.
