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

DIRECTOR OF GRADUATE STUDIES IN CHEMICAL ENGINEERING, 01/2010 – present
Department of Chemical Engineering and Materials Science, University of Minnesota

DIRECTOR, 01/01/03-present
University of Minnesota Summer Bioinformatics Institute

ASSISTANT PROFESSOR, 08/23/01-07/31/07
Department of Chemical Engineering and Materials Science, University of Minnesota
Digital Technology Center, University of Minnesota

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

- 2010 Thiele Lectureship, University of Notre Dame
- 2010 Charles Bowers Teaching Award, College of Science and Engineering, University of Minnesota
- 2009 AIChE Computing and Systems Technology Division Outstanding Young Researcher Award
- 2007 NSF CAREER Award
- 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)

Books

Yiannis N. Kaznessis, Statistical Thermodynamics and Stochastic Kinetics, an Introduction for Engineers, 2011, Cambridge University Press.

Research Publications
(pdf reprints available at www.cems.umn.edu/research/kaznessis/publications.htm)

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 Benzamidine-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 13C-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 dodecylphoshocholine 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.
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, YN. 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 hemolycity of protegrin-like antimicrobial peptides: Predicting experimental toxicity" Peptides, 2008, 29(7): 1085-1093.
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
51. Kaznessis YN. "Computational Methods in Synthetic Biology", Biotechnology Journal, 2009, in press,
52. Sayyed-Ahmad, A, Khandelia, H, Kaznessis YN. "Relative free energy of binding between antimicrobial peptides and SDS or DPC micelles", Molecular Simulation, 2009, 35(10–11):986–997,
53. Ramalingam, KI, Tomshine, JR, Maynard, JA, Kaznessis YN. " Forward engineering of synthetic bio-logical AND gates" Biochemical Engineering Journal, 2009, 47(1-3):38-47.
54. Magotti P, Ricklin D, Qu H, Wu YQ, Kaznessis YN, Lambris JD. " Structure-kinetic relationship analysis of the therapeutic complement inhibitor compstatin " J Mol Recognit . 2009, in press, link,

55. Mulakala, C; Kaznessis YN "Path-Integral Method for Predicting Relative Binding Affinities of Protein-Ligand Complexes" Journal of American Chemical Society, 2009 , 131 (12), 4521–45281.
56. Langham A, Kaznessis YN." Molecular simulations of antimicrobial peptides." Methods Mol Biol. 2010;618:267-85.
57. Kaznessis YN. Multiscale models for synthetic biology. Conf Proc IEEE Eng Med Biol Soc. 2009;1:6408-11.
58. Bolintineanu D, Hazrati E, Davis HT, Lehrer RI, Kaznessis YN. "Antimicrobial mechanism of pore-forming protegrin peptides: 100 pores to kill E. coli." Peptides. 2010, 2010, 31(1):1-8.
59. Sayyed-Ahmad A, Kaznessis YN. "Determining the orientation of protegrin-1 in DLPC bilayers using an implicit solvent-membrane model." PLoS One. 2009;4(3):e4799
60. Vivcharuk V, Kaznessis YN, "Free Energy Profile of the Interaction between a Monomer or a Dimer of Protegrin-1 in a Specific Binding Orientation and a Model Lipid Bilayer", J Phys Chem B, 2010, 114(8):2790-7.
61. Weeding E, Houle J, Kaznessis YN "SynBioSS Designer: A Web-Based Tool for the Automated Generation of Kinetic Models for Synthetic Biological Constructs Briefings in Bioinformatics, 2010, Jul;11(4):394-402.
62. Vivcharuk, V; Kaznessis, YN, "Dimerization of Protegrin-1 in Different Environments", International Journal of Molecular Sciences, 2011, 11(9):3177-3194.
63. Bolintineanu, D. Kaznessis YN, "Computational Studies of Protegrin Antimicrobial Peptides: A Review", Peptides, 2011, 32(1):188-201.
64. Contou-Carrere, MN; Sotiropoulos, V; Kaznessis, YN, Daoutidis, P, "Model Reduction of Multi-Scale Chemical Langevin Equations", Systems and Control Letters, 2011, 60(1), 75-86.
65. Qu, HC; Magotti, P; Ricklin, D; Wu l; Kaznessis YN; Lambris J. "Novel analogues of the therapeutic complement inhibitor compstatin with significantly improved affinity and potency", Molecular Immunology, 2011, 48(4), 481-489.
66. Sotiropoulos, V; Kaznessis, YN, "Analytical derivation of moment equations in stochastic chemical kinetics" Chemical Engineering Science, 2011, 66(3), 268-277.
67. Biliouris, K; Daoutidis, P; Kaznessis YN. "Stochastic Simulations of the Tetracycline Operon", BMC Bioinformatics, 2011, 5:9.

Invited and Keynote Presentations since 2007

- "Mathematical Modeling in Biological Engineering", Nara University, Nara, Japan, October **2011**.
- "Mathematical Modeling in Biological Engineering", Duke University, April **2011.**
- "Mathematical Modeling in Biological Engineering", Midwest Thermodynamics and Statistical Mechanics Conference, May **2011**, keynote.
- "Mathematical Modeling in Biological Engineering", Symposium in honor of Fred Heineken, AIChE Annual Meeting, Salt Lake, UT, November **2010**
- "Mathematical Modeling in Biological Engineering", University of Pittsburgh, October **2010**
- "Mathematical Modeling in Biological Engineering", MIT, September **2010**
- "Mathematical Modeling in Biological Engineering", Keynote speech, From Computational Biology to Systems Biology, May **2010**, Traverse City, MI
- "Computer-Aided Design of Synthetic Biological Systems", FNANO, April, **2010**, Snowbird, UT
- "High-Performance Computing in Synthetic Biology", March **2010**, New Delhi India, US-Indo Frontiers in Engineering conference
- "Multiscale Models for Synthetic Biology", Systems Biology GFST Symposium, June **2009**, Iowa State University, Ames Iowa
- "Multiscale Models for Synthetic Biology", Advances in Synthetic Biology, April **2009**, London, England
- "Computer-Aided Design of Antimicrobial Peptides", Gordon Conference on Antimicrobial Peptides, March **2009**, Anaheim, CA

- "Multiscale Models for Synthetic Biology", Rensselaer Polytechnic Institute, January **2009**.
- "Multiscale Models for Synthetic Biology", Princeton University, December **2008**.
- "Computer-Aided Synthetic Biology", International Conference of Systems Biology, August **2008**, Gothenburg, Sweden.
- "Computer-Aided Synthetic Biology", WORLDCOM 08, July **2008**, Las Vegas NV.
- "Computer-Aided Synthetic Biology", Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean Countries, May **2008**, Cetraro, Italy.
- "Synthetic Bio-logical AND gates", Pathways, Networks and Systems Biology, Porto Heli, Greece, July **2007**.

Conference Presentations since 2007

- V. Vivcharuk, D. S. Bolintineanu, Y. N. Kaznessis ``Multiscale models of antimicrobial peptides". 2011 Biophysical Society Annual Meeting, Baltimore, Maryland.
- V. Vivcharuk, Y.N. Kaznessis, ``Dimerization of Protegrin-1 Peptides in Different Environments". AIChE Annual Meeting, Salt Lake City, UT. November 2010.
- K. Biliouris, Daoutidis P., Kaznessis YN, "Stochastic Simulations of the Tetracycline Operon", AIChE Annual Meeting, Salt Lake, UT, November 2010.
- K. Volzing and Kaznessis Y. "Novel synthetic transcription regulators for prokaryotes," AIChE Annual Meeting. Salt Lake City, UT. November 2010.
- D. S. Bolintineanu, V. Vivcharuk, A. Langham, Y.N. Kaznessis ``Multiscale Computational Investigations of Antimicrobial Action". 2010 AIChE Annual Meeting. Salt Lake City, UT. November 2010.
- D. S. Bolintineanu, V. Vivcharuk, Y. N. Kaznessis "Statistical Mechanical Model of Antimicrobial Peptide Action: Peptide Aggregation, Membrane Adsorption and Membrane Insertion Equilibria" AIChE Annual Meeting. Salt Lake City, UT. November 2010.
- Y. Kaznessis, "From molecules to life: Multiscale models in biology", American Chemical Society, Boston, MA, August 2010.
- D. Bolintineanu, Y. Kaznessis, "How to protegrins kill bacteria. Molecular simulations", Midwest Thermodynamics conference, Notre Dame, IN, May 2010.
- K. Volzing, Sotiropoulos V, Kaznessis Y. "Novel tetracycline-inducible regulatory networks," Systems Biology: Integrative Comparative and Multi-Scale Modeling. Iowa State University at Ames. June 14, 2009.
- K. Volzing and Kaznessis Y. "Synthetic tetracycline-inducible transcription regulators," Global COE International Symposium, on the theme of Environmental Adaptation. NAIST at Nara, Japan. November 12-13, 2009.
- Y. Kaznessis, "From molecules to life: Multiscale models in biology", Midwest Thermodynamics conference, Notre Dame, IN, May 2010.
- V. Vivcharuk, D. Bolintineanu, Y. Kaznessis, "Computer simulations and free energy calculations of protein-DNA binding. Application to TetR:tetO system", American Institute of Chemical Engineers Annual Meeting, Nashville, TN, November 2009.
- K. Volzing, Y. Kaznessis, "Novel Synthetic Inducible Regulators", American Institute of Chemical Engineers Annual Meeting, Nashville, TN, November 2009.
- Y. Kaznessis, "From molecules to life: Multiscale models in biology", American Institute of Chemical Engineers Annual Meeting, Nashville, TN, November 2009.
- D. Bolintineanu, Y. Kaznessis, "How to protegrins kill bacteria. Molecular simulations", American Institute of Chemical Engineers Annual Meeting, Nashville, TN, November 2009.
- V. Sotiropoulos, Y. Kaznessis, "Integration schemes for stochastic differential equations", American Institute of Chemical Engineers Annual Meeting, Nashville, TN, November 2009.
- V. Vivcharuk, Y. Kaznessis, "Mechanism of protegrin dimerization. Insights from computer simulations", American Institute of Chemical Engineers Annual Meeting, Nashville, TN, November 2009.

- D. S. Bolintineanu, Ehsan Hazrati, Allison Langham, Rober I. Lehrer, H. Ted Davis, Yiannis N. Kaznessis. "Computational models of the action of protegrin antimicrobial peptides: transient ion diffusion and osmotic swelling." American Chemical Society 238th National Meeting, Washington, DC, August 2009.
- D. S. Bolintineanu, Yiannis N. Kaznessis and H. Ted Davis. "Modeling osmotic lysis of cells by antimicrobial peptides: transient diffusion of ions and osmotically-driven flow". Poster presentation, Biophysical Society Annual meeting, Boston, MA, March 2009.
- Y. Kaznessis and 10 Bioinformatics Summer Institute undergraduates, "Synthetic Bio-Logical AND gates", iGEM 2008, November 2008, Boston, MA.
- A. Langham, Y. Kaznessis "How do antimicrobial peptides work?", American Institute of Chemical Engineers Annual Meeting, Philadelphia, PA, November 2008.
- J Tomshine, K.I. Ramalingham, J.A. Maynard, Y. Kaznessis, "Bio-logical AND gates", American Institute of Chemical Engineers Annual Meeting, Philadelphia, PA, November 2008.
- D. Bolintineanu, V. Vivcharuk, A. Langham, Y. Kaznessis, "Multiscale modeling of electrodiffusion through antimicrobial peptide pores", American Institute of Chemical Engineers Annual Meeting, Philadelphia, PA, November 2008.
- J Tomshine, Y. Kaznessis, "Bio-logical AND gates", Synthetic Biology 4.0, October, 2008, Hong Kong, China.
- A. Langham, D. Bolintineanu, Y. Kaznessis, "How to protegrins kill bacteria. Molecular simulations", American Institute of Chemical Engineers Annual Meeting, Salt Lake, UT, November 2007.
- J. Tomshine, Y. Kaznessis, "Bio-logical AND gates", American Institute of Chemical Engineers Annual Meeting, Salt Lake, UT, November 2007.
- V. Sotiropoulos, Y. Kaznessis, "Hybrid stochastic differential equations", American Institute of Chemical Engineers Annual Meeting, Salt Lake, UT, November 2007.
- Y. Kaznessis, "Synthetic Bio-logical AND gates", Synthetic Biology 3.0, Zurich, Switzerland, 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.

Membership

American Institute of Chemical Engineers, American Chemical Society

Professional Activities - Service

- Director of Graduate Studies in Chemical Engineering, CEMS, 2010-
- Member, National Institutes of Health Study Section of Biodata Management and Analysis, 2010-
- Director, Area 15, AIChE, 2008-
- Chair of programming, Area 15c, AIChE, 2011
- Chair, Faculty Search Committee, CEMS 2009-2010
- Director, University of Minnesota Bioinformatics Summer Institute
- Editorial Board, BMC Systems Biology
- Chair, Steering Committee, Unisys/Minnesota Supercomputing Institute Alliance
- Fellow, Minnesota Supercomputing Institute
- ***Past service*:** Chair of programming, Area 10d, AIChE, 2009; Member, NSF Partnership for Advanced Computational Infrastructure Committee; Member, Internal Advisory Committee, Minnesota Supercomputing Institute; 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; 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, Kostas Billiouris, Ben Swiniarski, Patrick Smadbeck, Andrew Hirsch, Anushree Chatterjee

Postdoctoral Fellows: Fatemeh Ghasemi, Poonam Shrivastava, Victor Vivcharuk, Emilia Wu

Past Group Members

Dan Bolintineanu, (Ph.D. 2010) now postdoctoral fellow at the University of Minnesota
Vassilios Sotiropoulos (Ph.D. 2009) now serving in the Greek Army
Jonathan Tomshine (Ph.D. 2009) now at Solyndra.
Allison Langham (Ph.D. 2008) now at the Pentagon.
Spyros Vicatos (Ph.D. 2007) now research associate at the University of Southern California.
Howard Salis (Ph.D. 2007) now assistant professor at Penn State University.
Himanshu Khandelia (Ph.D. 2006) now research associate at the University of Southern Denmark
Nathan Ostberg (M.Sc), Lisa Tuttle (BSI and M.Sc.)
Abdallah Sayyed-Ahmad (postdoctoral fellow, now assistant professor at Berzeit University)
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)
Chandrika Mulakala (postdoctoral fellow)
Ting Lan Chiu (postdoctoral fellow)
Another four chemical engineering undergraduate students have worked in our group, along with seventeen Bioinformatics Summer Institute interns.