

Nikolaos Voulgarakis

Associate Professor

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Research Interests

Applied and computational mathematics with emphasis on stochastic processes, fluid dynamics, nonlinear dynamics, multiscale modeling, and numerical analysis.

Education

- 2003 Ph.D. Department of Physics, University of Crete, Greece
Thesis: “*Nonlinear Localization in Model Systems and Materials*”
Advisor: George Tsironis
- 2001 M.S. Department of Physics, University of Crete, Greece
- 1998 B.S. Department of Physics, University of Crete, Greece

Professional Experience

- Associate Professor of Mathematics since September 2018
Department of Mathematics, Washington State University
- Assistant Professor, August 2012 – August 2018
Department of Mathematics, Washington State University
- Research Associate, 2010 – 2012
Department of Chemical and Biochemical Engineering, University of California, Berkeley
- Postdoc, 2007 – 2010
Department of Chemical and Biochemical Engineering, University of California, Berkeley
- Postdoc 2005 – 2007
Center for Nonlinear Studies, Los Alamos National Laboratory
- Visiting Assistant Professor, 2003 – 2005
Department of Physics, University of Crete, Greece

Grants

- “*Modeling Nanoscale Fluid-Structure Interfaces*,” NSF - DMS (PI, \$151,000, 2014-2018)

- “Hybrid Molecular and Continuum Mechanics for Nanoscale Modeling of Gene Delivery,” Washington State University - New Faculty Grant. (PI, \$29,000, 2013-2014)
- Washington State University - Chancellor’s equipment grant (PI, \$5,000, 2014-2015)
- “Gene Therapy: Modeling Synthetic DNA Delivery Systems,” Marie Curie reintegration grant, EU (PI, €100,000, 2009). PI declined this grant for personal reasons.

Awards and Scholarships

- National Scholarship Foundation Award for outstanding performance in the first year of the graduate program (1999)
- University of Crete Award for outstanding performance in the second year of the graduate program (2001)
- Full time scholarship from the Institute of Electronic Structure and Laser (I.E.S.L) of the Foundation for Research and Technology-Hellas (FO.R.T.H) and the University of Crete for postgraduate and Ph.D. studies (1998-2003)

Publications

(* graduate student, ** undergraduate student. NOTE: In most of the journals below, the last author usually refers to the PI)

Submitted/Published Manuscripts:

1. “A stochastic reaction-diffusion model for protein aggregation on DNA,” N. K. Voulgarakis *Int. J. Mod. Phys. C*, **28**, 1 (2017)
2. “A hybrid fluctuating hydrodynamics and kinetic Monte Carlo method for modeling chemically-powered nanoscale motion,” S. Selmi*, D. Mitchell, V. Manoranjan, and N. K. Voulgarakis *J. Math. Chem.*, **55**, 1833 (2017)
3. “The effect of thermal fluctuations on Holstein polaron dynamics in electric field,” N. K. Voulgarakis, *Physica B*, **516**, 15 (2017)
4. “Fluctuating hydrodynamics for ionic liquids,” K. Lazaridis*, L. Wickham**, and N. K. Voulgarakis, *Phys. Lett. A*, **381** (16), 1431 (2017)
5. “A two-level stochastic collocation method for semilinear elliptic equations with random coefficients,” L. Chen, B. Zheng, G. Lin, and N. K. Voulgarakis, *J. Comput. Appl. Math.*, **315**, 195 (2017)
6. “Modeling nanoscale hydrodynamics by smoothed dissipative particle dynamics,” H. Lei, C. J. Mundy, G. K. Schenter, and N. K. Voulgarakis, *J. Chem. Phys.*, **142**, 194504 (2015)

7. "Allostery through protein-induced bubbles," J. Traverso**, V. Manoranjan, K. Rasmussen, A. R. Bishop, and N. K. Voulgarakis, *Scientific Reports*, **5**, 9037 (2015) - doi:10.1038/srep09037
8. "Dynamic mesoscale model of dipolar fluids via fluctuating hydrodynamics," R. A. X. Person, N. K. Voulgarakis and J-W. Chu, *J. Chem. Phys.*, **141**, 174105 (2014)
9. "Linking hydrophobicity and hydrodynamics by the hybrid fluctuating hydrodynamics and molecular dynamics methodologies," N. K. Voulgarakis, B. Shang, and J-W. Chu, *Phys. Rev. E* **88**, 023305 (2013)
10. "Fluctuating hydrodynamics for multiscale modeling and simulation: Energy and heat transfer in molecular fluids," B. Shang, N. K. Voulgarakis, and J-W. Chu, *J. Chem. Phys.*, **137**, 044117 (2012)
11. "Fluctuating hydrodynamics for multiscale simulation of inhomogeneous fluids - Mapping all-Atom molecular dynamics to capillary waves," B. Shang, N. K. Voulgarakis, and J-W. Chu, *J. Chem. Phys.*, **135**, 044111 (2011)
12. "Modeling the viscoelasticity and thermal fluctuations of fluids at the nanoscale," N. K. Voulgarakis, S. Satish, and J-W. Chu, *Molecular Simulation*, **131**, 552 (2010)
13. "Modeling the nanoscale viscoelasticity of fluids by bridging non Markovian fluctuating hydrodynamics and molecular dynamics simulations," N. K. Voulgarakis, S. Satish, and J-W. Chu, *J. Chem. Phys.*, **131**, 234115 (2009)
14. "Dendrimers as gene delivery vectors: cell membrane attachment," N. K. Voulgarakis, K. Ø. Rasmussen, P. M. Welch, *J. Chem. Phys.*, **130**, 155101 (2009)
15. "Bridging fluctuating hydrodynamics and molecular dynamics simulations of fluids," N. K. Voulgarakis and J.-W. Chu, *J. Chem. Phys.*, **130**, 134111 (2009)
16. "Pre-melting dynamics of DNA and its relation to specific functions," B. Alexandrov, N. K. Voulgarakis, K. Ø. Rasmussen, A. Usheva, and A. R. Bishop, *J. Phys.: Condensed Matter*, **21**, 034107 (2009)
17. "Opening rates of DNA hairpins: experiment and model," J. Hanne, G. Zocchi, N. K. Voulgarakis, A. R. Bishop, and K. Ø. Rasmussen, *Phys. Rev. E*, **76**, 011909 (2007)
18. "Sequencing DNA by dynamic force spectroscopy: limitations and prospects," N. K. Voulgarakis, A. Redondo, A. R. Bishop, and K. Ø. Rasmussen, *Nano Lett.*, **6**, 1483 (2006)
19. "Probing the mechanical unzipping of DNA," N. K. Voulgarakis, A. Redondo, A. R. Bishop, and K. Ø. Rasmussen, *Phys. Rev. Lett.*, **96**, 248101 (2006)
20. "Bubble nucleation and cooperativity in DNA melting," S. Ares, N. K. Voulgarakis, K. Ø. Rasmussen, and A. R. Bishop, *Phys. Rev. Lett.*, **94**, 035504 (2005)
21. "Temperature-dependent signatures of coherent vibrational openings in DNA," N. K. Voulgarakis, G. Kalosakas, K. Ø. Rasmussen, and A. R. Bishop, *Nano Lett.*, **4(4)**, 629

(2004)

22. “Computational investigation of intrinsic localization in crystalline Si,” N. K. Voulgarakis, G. Hadjisavvas, P. C. Kelires, and G. P. Tsironis, *Phys. Rev. B*, **69**, 113201 (2004)
23. “Thermally induced coherent vibrations in DNA,” K. Ø. Rasmussen, G. Kalosakas, N. K. Voulgarakis, A. R. Bishop, C. H. Choi, and A. Usheva, *Proceedings of SPIE - The International Society for Optical Engineering*, 5467, 235 (2004)
24. “Polaronic electron transfer in β -sheet protein models,” N. K. Voulgarakis, D. Hennig, H. Gabriel, and G. P. Tsironis, *J. Phys.: Condens. Matter*, **13**, 9821 (2001)
25. “Multiquanta breather model for PtCl,” N. K. Voulgarakis, G. Kalosakas, A. R. Bishop, and G. P. Tsironis, *Phys. Rev. B*, **64**, R020301, (2001)
26. “Stationary and dynamical properties of polarons in the anharmonic Holstein model,” N. K. Voulgarakis and Tsironis, *Phys. Rev. B*; **63**, 014302 (2001)
27. “Energy relaxation in discrete nonlinear lattices,” A. Bikaki, N. K. Voulgarakis, S. Aubry, and G. P. Tsironis, *Phys. Rev. E*, **59**, 1234 (1999)

Book Chapters

1. “Modeling Interactions in Learning Settings and their Impact on the Learning Process. Distance and E-Learning in Transition,” G. Neofotistos, N. Kastis, E. Tsourlidaki, N. K. Voulgarakis, **284**, 711–720 (John Wiley & Sons, Inc., 2013).

Press Releases

- Science Daily, May 13th, 2009, “*First Large-scale Computer Simulation Of Gene Therapy*”
- Biomedical Computation Review, Fall, 2009, “*Modeling a Gene Therapy Delivery Vehicle*”
- Vertical News Physics, May 26th, 2009, “*Study results from University of California update understanding of chemical physics*”
- Los Alamos National Lab. News Letter, December 4th, 2006, “*Unzipping the Molecule of Life*”

Reviewer

- NSF: Scalable Nano-Manufacturing Program
- Biophysical Journal
- Applied Mathematics

- Nano Letters
- Journal of Chemical Physics
- Physical Review Letters
- Physical Biology
- Physics Letters A
- Physical Review E
- International Journal of Modern Physics C
- European Physical Journal
- Communications in Nonlinear Science and Numerical Simulation

Member of Editorial Board for Peer-Reviewed Journals

- Scientific Reports (*Nature Publishing Group*)

Invited Talks

- “*Fluctuating Hydrodynamics for Ionic Liquids*,” 2018 SIAM Conference on Mathematical Aspects of Materials Science, Portland, OR, July 2018
- “*Modeling Reversible Protein Aggregation on DNA and Its Impact on Gene Compaction*,” 2018 SIAM Conference on Mathematical Aspects of Materials Science, Portland, OR, July 2018
- “*Allostery through Protein-induced DNA Bubbles*,” 19th Annual Meeting of the Northwest APS Section, Tacoma, WA, June 2018
- “*The impact of allostery on mitochondrial DNA packaging*,” Physics Colloquium, University of Idaho, ID, April 2018
- “*Mathematical Modeling of DNA Allostery*,” Mathematical Biology Seminar, Washington State University, WSU, November 2017
- “*Mathematical Modeling of DNA Allostery*,” Mathematical Biology Seminar, Washington State University, WSU, February 2017
- “*Modeling the Effect of Hydrophobicity on Nanoparticle Suspensions*,” 2016 SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA, May 2016 (not able to travel due to health issues)
- “*Hybrid Methodologies for Nanoscale Fluid-Solid Interaction*,” CECAM workshop: Virus as a whole: meso- and macroscopic structure and dynamics at all atom resolution, Lausanne, Switzerland, October 2015
- “*Modeling Fluid-Structure Interfaces at the Nanoscale*,” CECAM workshop: Fluctuating Hydrodynamics meets Molecular dynamics, Madrid, Spain, May 2015
- “*Modeling Nanoscale Fluid-Solid Interfaces*,” 2014 SIAM Annual Meeting, Chicago, IL, June 2014

- “*Coupling Fluid and Molecular Mechanics for Nanoscale Simulations of Soft Matter,*” *Math Colloquium, University of Idaho, ID,* October 2013
- “*Linking Hydrophobicity and Hydrodynamics for Nanoscale Simulations of Soft Matter,*” 7th Sino-US Joint Conference of Chemical Engineering, Beijing, China, October, 2013
- “*Coupling Fluctuating Hydrodynamics with Molecular Dynamics at the Nanoscale,*” APS March Meeting 2011, Dallas, TX, 2011
- “*Coupling Molecular and Field Mechanics for Multiscale Modeling of Soft Matter,*” Tufts University, Department of Physics, February 16, 2011
- “*A Combined Fluctuating Hydrodynamics and Molecular Dynamics Method for Simulating Complex Molecular Systems at the Nanoscale,*” AIChE Annual Meeting, Salt Lake City, UT, 2010
- “*Unzipping DNA,*” University of Pittsburgh, Medical School, November 15, 2006
“*Mechanical Denaturation of DNA,*” Cornell University, Medical School, November 7, 2006
- “*Dynamics of Double Stranded DNA,*” International Annual Workshop "Dynamics Days Europe 2006" Greece, September 25-29, 2006
- “*Unzipping DNA,*” University of California, Department of Physics, Los Angeles (UCLA) September 20 2006
- “*Dynamics of Double Stranded DNA,*” The 2nd International Workshop on "The Nanoelectronics and Dynamics of DNA" Maui, HI, August 20-22, 2006
- “*Energy Localization in PtCl,*” University of Zurich, Department of Physics, February 20, 2004

Advising Experience

Students supervising at the Department of Mathematics and Statistics, Washington State University:

- **Graduate students**
 - Kellan Tomen, Ph.D. candidate, Mathematics (expected 2019)
 - Konstantinos Tsampourakis, Ph.D. candidate, Mathematics (expected 2022)
 - Konstantinos Lazaridis, M.S. Applied Mathematics (2016)
 - Saranah Selmi, Ph.D. candidate, Engineering Science (2018)
- **Undergraduate students**
 - Hayden Arch (Stochastic Dynamics, 2018-present)
 - Grant Hutchings (Fluid Dynamics, 2016-2017)
 - Logan Wickham (Fluid Dynamics, 2015)

- Daniel Herrera (DNA allostery, 2014)
- Joseph Traverso (protein-DNA interaction and DNA allostery, 2013-2014)
- **Undergraduate research fellowships and awards for students worked on my projects**
 - *Auwil Scholarship*: Joseph Traverso (2013), Logan Wickham (2015), Hayden Arch (2018)
 - *Carson Scholarship*: Joseph Traverso (2014)
 - *Louis Stokes Alliance for Minority Participation (LSAMP)*: Daniel Herrera (2014)
 - *Chancellor's summer scholarship*: Joseph Traverso (2014)
 - First Award in "Computer Science, Mathematics, Statistics, and Information Sciences" category at Showcase for Undergraduate Research and Creative Activities (SURCA), WSU: Daniel Herrera (2015)
 - First Award in "Computer Science, Mathematics, Statistics, and Information Sciences" category at SURCA, WSU: Joseph Traverso (2014)
- **Undergraduate students who published in peer review journals**
 - Joseph Traverso (2015)
 - Logan Wickham (2017)
- **Graduate Committees**
Served as a committee member for 5 Ph.D. and 2 Master's students

Teaching Experience

Courses Taught in the Department of Mathematics and Statistics, Washington State University:

- MATH 315: Differential Equations (Spring 2013, 2014, 2015, 2016, 2017, and Fall 2016)
- MATH 140: Calculus for Life Sciences (Spring 2013, 2014, 2015 and Fall 2017)
- MATH 440/540: Applied Mathematics I (Fall 2012, 2013, 2014)
- MATH 170: Calculus I (Spring 2016)
- STAT 544: Applied Stochastic Processes (Spring 2017, 2019)
- MATH 512: Applied Stochastic Processes (Fall 2018)
- MATH 486/586: Mathematical Modeling in Life Sciences (Fall 2018)