EVANGELIA KALLIGIANNAKI

Research Scientist
Stochastic Numerics Research Group
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EDUCATION

Ph.D. in Applied Mathematics, 2007
Department of Applied Mathematics, University of Crete, Greece.
Advisor: George N. Makrakis.
Thesis title: *Asymptotic solutions of the Wigner equation and high-frequency wave propagation near caustics.*

M.S. in Applied Mathematics, 2002
Department of Mathematics, University of Crete, Greece.
Thesis title: *The particle method for the Wigner equation in high frequency paraxial propagation.*

B.Sc. in Mathematics, 1999
Department of Mathematics, University of Crete, Greece.
Thesis title: *Computation of high-frequency fields near cusp caustics.*

PROFESSIONAL EXPERIENCE

Research scientist 2016 - today
Computer, Electrical and Mathematical Sciences & Engineering,
King Abdullah University of Science and Technology (KAUST).
Stochastic sampling and inference for particle systems and reaction networks.
Multi-level and Multi-index Monte Carlo methods.

Post-doctoral research associate 2013 - 2015
Department of Mathematics & Applied Mathematics
University of Crete.
Multiscale modeling and analysis for complex molecular systems at and out of equilibrium.

Post-doctoral research associate 2012 - 2013
Department of Aerospace & Mechanical Engineering
University of Southern California.
Stochastic models with uncertainty using polynomial chaos expansions.

Post-doctoral research associate 2009 - 2012
Oak Ridge National Laboratory & University of Tennessee,
Department of Mathematical Sciences, University of Delaware
and Department of Mathematics & Statistics
University of Massachusetts.
Analysis, development and implementation of algorithms for simulations of stochastic multi-scale particle systems with Monte Carlo methods.

Post-doctoral research associate 2007- 2009
Institute of Applied & Computational Mathematics
Foundation for Research & Technology- Hellas.
Mean field theory for polymer systems via Large Deviations theory.

Research assistant 1999
Institute of Applied & Computational Mathematics,
Foundation for Research & Technology- Hellas.

RESEARCH INTERESTS

Multi-scale modeling. Uncertainty quantification. Variational inference. Statistical mechanics. Stochastic simulations. Markov chain Monte Carlo methods. Multi-level & Multi-Index Monte Carlo methods. Interacting particle systems. Complex fluids and polymers. Surface processes. Semiclassical asymptotics, high frequency fields near caustics.

PUBLICATIONS

1. E. Kalligiannaki, A. Chazirakis, A. Tsourtis, M. Katsoulakis P. Plechac and V. Harmandaris, *Parametrizing coarse grained models for molecular systems at equilibrium*, EPJ ST, 225(8), 1347-1372, 2016, DOI: 10.1140/epjst/e2016-60145-x.

2. V. Harmandaris, E. Kalligiannaki, M. Katsoulakis and P. Plechac, *Path-space variational inference for non-equilibrium coarse-grained systems*, J. Comp. Phys., 314(1), 355–383, 2016, DOI: 10.1016/j.jcp.2016.03.021.

3. E. Kalligiannaki, V. Harmandaris, M. Katsoulakis and P. Plechac, *The geometry of force matching in coarse graining and related information metrics*, J. Chem. Phys., 143, 084105, 2015, DOI: 10.1063/1.4928857.

4. E. Kalligiannaki, M. Katsoulakis and P. Plechac. *Spatial two-level interacting particle simulations and information theory-based error quantification*, SIAM J. Sci. Comput. 36(2), A634–A667, 2014, DOI: 10.1137/120887060.

5. E. Kalligiannaki, M. Katsoulakis, P. Plechac and D. Vlachos. *Multilevel coarse graining and nanopattern discovery in many particle stochastic systems*. J. Comp. Phys., 231(6), 2599–2620, 2012, DOI: 10.1016/j.jcp.2011.12.011.

6. E. Kalligiannaki, M. Katsoulakis and P. Plechac. *Coupled coarse graining and Markov Chain Monte Carlo for lattice systems*. "Numerical Analysis of Multiscale Computations", Eds: B. Engquist, O. Runborg, Y R. Tsai, Lect. Notes Comput. Sci. Eng. 82, 2011, 235–257, 2012, DOI: 10.1007/978-3-642-21943-6_11.

7. E. Kalligiannaki, G.N. Makrakis. *Conservation equations for the semiclassical Schrodinger equation near caustics.* Applicable Analysis, 86(8), 2007, 917– 944, DOI: 10.1080/00036810701355000 .

8. E. Kalligiannaki, Th. Katsaounis and G.N. Makrakis. *High frequency waves near cusp caustics.* Quarterly of Applied Mathematics, 61(1), 111–129, 2003.

WORK IN PROGRESS

1. C. Ben Hammouda, E. Kalligiannaki, R. Tempone, P. Vilanova,
   Multi-Index Monte Carlo for complex Stochastic Reaction Networks with applications in breakage and coagulation processes.

2. S. Elkantassi, E. Kalligiannaki, R. Tempone,
   Moment matching and indirect inference with partially observed states.

3. S. Elkantassi, E. Kalligiannaki, R. Tempone,
   Inference and sensitivity for stochastic wind power generation models.

PRE-PRINTS

1. E. Kalligiannaki, G.N. Makrakis. *Perturbation solutions of the semiclassical Wigner equation*, preprint arXiv:1402.6194.

THESES

1. E. Kalligiannaki (2007). Asymptotic solutions of the Wigner equation and high frequency wave propagation near caustics. Ph.D. thesis, University of Crete, Greece.

2. E. Kalligiannaki (2002). The particle method for the Wigner equation in high frequency paraxial propagation. Master thesis, University of Crete, Greece.

3. E. Kalligiannaki (1999). Computation of high frequency fields near cusp caustics. Diploma thesis, University of Crete, Greece.

MEMBERSHIP Society of Industrial and Applied Mathematics, SIAM.

LANGUAGES English (fluent), German (basic), Greek (native).

COMPUTING SKILLS FORTRAN, JAVA, C++, MATLAB.

TEACHING

Co-supervisor of master thesis.
KAUST. in progress
Simulations and Inference in Stochastic Reaction Networks.

Co-supervisor of undergraduate diploma thesis.
University of Crete. 2014-2015
Minimization of Relative Entropy Rate for numerical schemes of Langevin equations.

Instructor.
University of Southern California (USC). Spring 2013
Calculus II.

Reading seminar instructor.
UQ group seminar, USC. Fall 2012
Gaussian Hilbert spaces.

Co-supervisor of graduate research assistant, 2011-2012
University of Delaware.
Markov chain Monte Carlo methods and coarse graining.

Lecture series instructor, JICS/ORNL. Summer 2010
Lectures on Markov chain Monte Carlo methods.

Teaching Assistant, University of Crete. 1999-2006
Probability theory, Statistics, Calculus I, Calculus II,
Introduction to Computing, Mathematical Modeling,
Optimization theory, Foundations of Mathematics.

Teaching Assistant. 2002-2003
Technological & Educational Institute of Crete.
Calculus for electrical engineering I.

AWARDS & GRANTS

AWM - NSF Travel Award
7th International Congress on Industrial and Applied Mathematics - ICIAM 2011, Canada.

IKY (State Scholarships Foundation), Postdoctoral research scholarship, Greece 2009 (rejected).

Clay Mathematics Institute, Travel Award, 2008 Summer School *Evolution Equations*
ETH Swiss Federal Institute of Technology, Zurich, Switzerland, June 23 - July 18 2008

Manassaki Scholarship, Department of Applied Mathematics, University of Crete Oct 2006-Sept 2007.

Ph.D. Fellowship *"Herakleitos"*, grant funded by the Greek Ministry of National Education and the European Commission, 2002–2006.

Graduate Fellowship, Institute of Applied and Computational Mathematics, Foundation for Research and Technology Hellas 1999- 2002.

PRESENTATIONS (selected list)

- European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2016), Crete Island, Greece, June 5-10, 2016.
- Transferability Issues in Multiscale Modeling of Hierarchical Phenomena, IRTG mini-workshop, Max Planck Institute for Polymer Research Mainz, Dec 7, 2015.
- Mathematical and Computational Techniques for Molecular Systems, Institute of Applied and Computational Mathematics, FORTH, & ACMAC Center, University of Crete, Heraklion 16-18 September 2015.
- 7th International Workshop and Summer School on Nonequilibrium Thermodynamics (IWNET 2015), Hilvarenbeek, Netherlands July 5-10, 2015.
- 1st International Conference on Uncertainty Quantification in Computational Sciences and Engineering (UNCECOMP 2015), Crete Island, Greece, May 25-27, 2015.
- MCM3: Multiscale Computational Methods in Materials Modeling Meeting. Edinburgh, June 18 - 20, 2014.
- Workshop on Numerical Analysis of Stochastic PDE's. EPFL, Lausanne, September 9 - 10, 2014.
- SIAM Conference on Computational Science & Engineering (CSE13), Boston, MA, February 25-March 1, 2013.
- Uncertainty Quantification, ICERM Semester Program on Computational Challenges in Probability. Providence, RI, October 9-13, 2012.
- 7th International Congress on Industrial and Applied Mathematics - ICIAM 2011. Vancouver, BC, Canada, July 18-22, 2011.
- Coarse-graining of many-body systems: analysis, computations and applications. Archimedes Center for Modeling, Analysis & Computation. Heraklion, Greece, June 27-July 1, 2011.
- The ACMAC workshop on Stochastic Partial Differential Equations
  Archimedes Center for Modeling, Analysis & Computation. Heraklion, Greece, June 13-17, 2011.
- SIAM Conference on Mathematical Aspects of Materials Science.
  Philadelphia, May 23-26, 2010.
- Numerical Analysis of Multiscale Computations.
  Banff International Research Station for Mathematical Innovation and Discovery, December 6 - 11, 2009.
- Second School and Workshop on Mathematical Methods in Quantum Mechanics. Bressanone (Italy), February 26 - March 3, 2007.