

CURRICULUM VITAE

Evangelia Kalligiannaki

Associate professor
Department of Statistics and Actuarial-Financial Mathematics,
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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*
Principal Investigator, Hellenic Foundation for Research and Innovation (H.F.R.I.), 2018- 2022
Institute of Applied and Computational Mathematics
Foundation for Research and Technology-Hellas, Greece
- Research projects for postdoctoral researchers.*
Project: Statistical Inference with Stochastic Differential Equations and applications in Complex Stochastic systems (SISDECS).
- Research scientist 2016 - 2018
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. <i>Analysis, development and implementation of algorithms for simulations of stochastic multi-scale particle systems with Monte Carlo methods.</i>	
Post-doctoral research associate	2007- 2009
Institute of Applied & Computational Mathematics Foundation for Research & Technology- Hellas. <i>Mean field theory for polymer systems via Large Deviations theory.</i>	
Research assistant	1999
Institute of Applied & Computational Mathematics, Foundation for Research & Technology- Hellas.	

RESEARCH INTERESTS

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

PUBLICATIONS

1. G. Baxevari, V. Harmandaris, E. Kalligiannaki, I. Tsantili. *Bottom-up transient time models in coarse-graining molecular systems*. Accepted SIAM MMS, 2023, preprint arXiv:2302.05159
2. Y. Pantazis, E. Kalligiannaki, Y. Kamarianakis, K. Kotsovos, I. Gereige, M. Abdullah, A. Jamal, A. Tzavaras and T. Katsaounis, *Efficiency evaluation and comparisons of solar cell technologies based on measurements from the Arabian peninsula*, EuroSun, 2022
3. Y. Kamarianakis, Y. Pantazis, E. Kalligiannaki, T. Katsaounis, K. Kotsovos, I. Gereige, M. Abdullah, A. Jamal, and A. Tzavaras, *KNN-based ensembles for day-ahead solar power output forecasting*, EuroSun, 2022
4. Y. Pantazis, E. Kalligiannaki, Y. Kamarianakis, K. Kotsovos, I. Gereige, M. Abdullah, A. Tzavaras, and T. Katsaounis, *Performance evaluation and comparison of solar cell technologies based on historical data*, 8th World Conference on Photovoltaic Energy Conversion, 2022
5. Y. Kamarianakis, Y. Pantazis, E. Kalligiannaki, K. Kotsovos, I. Gereige, M. Abdullah, A. Tzavaras and T. Katsaounis, *Day-ahead forecasting of solar irradiance: KNN-based ensembles*, 8th World Conference on Photovoltaic Energy Conversion, 2022
6. A. Chazirakis, V. Kirieri, E. Kalligiannaki, V. Harmandaris. *Neural Network Potential Surfaces: A comparison of two approaches*. Procedia Computer Science, 178, 345-354, 2020. DOI:10.1016/j.procs.2020.11.036
7. T. Jin, A. Chazirakis, E. Kalligiannaki, V. Harmandaris, and M. Katsoulakis *Data-driven Uncertainty Quantification for Systematic Coarse-grained Models*. Soft Materials, 18:2-3, 348-368, DOI: 10.1080/1539445X.2020.1765803, arXiv:2007.00340

8. E. Kalligiannaki, V. Harmandaris, and M. Katsoulakis, *Systematic Coarse-Grained Models for Molecular Systems Using Entropy*. Proceedings 2020, 46(1), 27 DOI: 10.3390/ecea-5-06710. 5th International Electronic Conference on Entropy and Its Applications.
9. G. Baxevas, E. Kalligiannaki, V. Harmandaris. *Study of the transient dynamics of coarse-grained molecular systems with the path-space force-matching method*. Procedia Computer Science, 156, 59-68, 2019.
10. V. Harmandaris, E. Kalligiannaki, M. A. Katsoulakis *Computational Design of Complex Materials Using Information Theory: from Physics-to Data-driven Multi-scale Molecular Models*, ERCIM News 115, 19-20, 2018.
11. E. Kalligiannaki, M. Katsoulakis and P. Plechac, V. Harmandaris. *Path space force matching and relative entropy methods for coarse-graining molecular systems at transient regimes*. Procedia Computer Science, 136, 331-340, 2018.
12. S. Elkantassi, E. Kalligiannaki and R. Tempone. *Inference and sensitivity for stochastic wind power forecast models*. UNCECOMP 2017, 2nd ECCOMAS Thematic Conference on Uncertainty Quantification in Computational Sciences and Engineering, Rhodes Island, Greece, 15-17 June 2017. DOI: 10.7712/120217.5377.16899
13. V. Harmandaris, E. Kalligiannaki, M. Katsoulakis and P. Plechac. *From Atomistic to Systematic Coarse-Grained Models for Molecular Systems*. UNCECOMP 2017, 2nd ECCOMAS Thematic Conference on Uncertainty Quantification in Computational Sciences and Engineering, Rhodes Island, Greece, 15-17 June 2017. . DOI: 10.7712/120217.5378.17211
14. 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.
15. 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.
16. 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.
17. 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.
18. E. Kalligiannaki, M. Katsoulakis, P. Plechac and D. Vlachos. *Multilevel coarse graining and nano-pattern discovery in many particle stochastic systems*. J. Comp. Phys., 231(6), 2599–2620, 2012, DOI: 10.1016/j.jcp.2011.12.011.
19. 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.
20. 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 .
21. E. Kalligiannaki, Th. Katsaounis and G.N. Makrakis. *High frequency waves near cusp caustics*. Quarterly of Applied Mathematics, 61(1), 111–129, 2003.

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.

AWARDS & GRANTS

- Hellenic Foundation for Research and Innovation (H.F.R.I.), 2018
Research projects for postdoctoral researchers.
Funding: 170.000 €.
Project: *"Statistical inference with stochastic differential equations and applications in complex stochastic systems"*.
- 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.

TEACHING & SUPERVISING

Teaching

<i>Stochastic processes</i> (undergraduate). Instructor. University of Crete.	Spring 2021
<i>Statistical Inference and Machine Learning with applications in Physical Sciences</i> (graduate). Instructor. (joint with Vagelis Harmandaris), University of Crete.	Spring 2020
<i>Calculus II</i> . Instructor. University of Southern California (USC).	Spring 2013

<i>Gaussian Hilbert spaces.</i> Reading seminar instructor. UQ group seminar, USC.	Fall 2012
<i>Lectures on Markov chain Monte Carlo methods.</i> Lecture series instructor, JICS/ORNL.	Summer 2010
Teaching Assistant, University of Crete. <i>Probability theory, Statistics, Calculus I, Calculus II,</i> <i>Introduction to Computing, Mathematical Modeling,</i> <i>Optimization theory, Foundations of Mathematics.</i>	1999-2006
<i>Calculus for electrical engineering I.</i> Teaching Assistant. Technological & Educational Institute of Crete.	2002-2003

Supervising

PostDoc

<i>Ivi Tsantili</i>	2020-today
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PhD

<i>Georgia Baxevasi. Dynamics of coarse-grained systems.</i> University of Crete.	2019-today
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Master

<i>Georgia Baxevasi. Development of coarse-grained models for the dynamics of molecular systems, through atomistic simulation data analysis.</i> University of Crete.	2018
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<i>Sofianna Kavousanou. Coarse-graining through Bayesian statistics.</i> University of Crete.	2015-2017
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<i>Soumaya Elkantassi. Simulations and Inference in stochastic systems.</i> KAUST.	2016-2017
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Co-supervisor of graduate research assistant, University of Delaware. <i>Markov chain Monte Carlo methods and coarse graining.</i>	2011-2012
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Undergraduate thesis

<i>Vasiliki Kirieri. Machine Learning Methods for parameterizing molecular models</i> University of Crete.	2019-2020
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<i>Eleutheria Stavropoulou. Dynamics of coarse graining systems. The generalized Langevin equation.</i> University of Crete. 2018-2019 <i>Alexia Katsara. Minimization of Relative Entropy Rate for numerical schemes of Langevin equations.</i> University of Crete.	2014-2015
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Internships

Ilias Sarris

Institute of Applied and Computational Mathematics - FORTH,

July 2020 -

Vasiliki Kirieri.

Institute of Applied and Computational Mathematics - FORTH,

February 2020 - April 2020

Korina Argyropoulou. Stochastic Landau-Lifshitz-Gilbert equation and applications.

Institute of Applied and Computational Mathematics - FORTH, December 2018 - February 2019

Menelaos Ampartzakis. Stochastic Landau-Lifshitz-Gilbert equation and applications.

Institute of Applied and Computational Mathematics - FORTH,

April-July 2018

MEMBERSHIP

Society of Industrial and Applied Mathematics, SIAM.
European Mathematical Society, EMS.

LANGUAGES

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

COMPUTING SKILLS

Python, FORTRAN, JAVA, C++, MATLAB.

PARTICIPATION IN CONFERENCES, WORKSHOPS & SCHOOLS (selected list)

- UNCECOMP 2021, 4th International Conference on Uncertainty Quantification in Computational Sciences and Engineering, 27-30 June 2021, Athens, Greece (online).
Organizing Mini-symposium "MS 4 Advances in data-driven modeling and applications ", with Dionissios Hristopoulos and Ivi Tsantili.
- SIAM Conference on Mathematical Aspects of Materials Science, May 17- 28 2021 online.
Organizing Mini-symposium "MS50: Physics based and data-driven multiscale materials modelling", with Vagelis Harmandaris and Markos Katsoulakis.
- DRIVEN Workshop on Digital Twins, Belval, Luxemburg, 11-12 September 2019
- EUROMAT 2019 - European Congress and Exhibition on Advanced Materials and Processes - Stockholm, Sweden, September 1-5, 2019. (Keynote lecture)
- 8th International Young Scientists Conference in Computational Science, Heraklion, Greece June 24-28, 2019. (Keynote lecture) UNCECOMP 2019 - 3rd International Conference on Uncertainty Quantification in Computational Sciences and Engineering, Crete, Greece, June 24-26, 2019 (Keynote lecture)
- ERCIM workshop on Digital Twins, Gothenborg, Sweden, 8-9 October 2018.
- Numerical analysis for deterministic and stochastic differential equations, School of Applied Mathematical and Physical Sciences of the National Technical University of Athens (NTUA), Athens, Greece, 10-13 July 2018.

- Stochastic Methods in Finance and Physics, FORTH, Heraklion, Crete, Greece, 23-27 July 2018.
- 7th International Young Scientists Conference in Computational Science, Heraklion, Crete, Greece, 2 - 6 July 2018.
- 2nd International Conference on Uncertainty Quantification in Computational Sciences and Engineering (UNCECOMP 2017), Rhodes Island, Greece, 15-17 June 2017.
- Uncertainty Quantification Summer School, WIAS, Berlin, September 2016.
- International Conference on Monte Carlo techniques, Paris, France, July 5 - 8th 2016.
- European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2016), Crete Island, Greece, June 5-10, 2016.
- Uncertainty Quantification School on Numerical Methods for Direct and Inverse Problems, KAUST, Thuwal, Saudi Arabia, May 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.