Vangelis Harmandaris

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Nicosia, Cyprus

Research Interests

Mathematical Modeling and Machine Learning: Mathematical/Big-data coarse-graining, stochastic processes, Bayesian statistics, applied probability, optimization algorithms, non-equilibrium methods, information metrics, statistical methods for analysis of big data, inverse problems.

Computational Modeling and Engineering: Hierarchical multi-scale modeling, atomistic simulations, mesoscopic modeling, molecular dynamics, Monte Carlo methods, Stochastic Brownian dynamics, field theory simulations, ab-initio DFT calculations, Non-equilibrium simulations.

Soft Condensed Matter: Structure-property relations, hybrid complex systems, polymers, biomolecular systems, biological membranes, self-assembled monolayers (SAMs), proteins, colloids.

Statistical Mechanics: thermodynamics, non-equilibrium thermodynamics.

Complex Polymeric Materials: Rheology and microscopic modelling, fluid-flow deformation dynamics, polymer nanocomposites, polymer/solid interfaces, thin polymer films, graphene-based polymeric systems.

Professional Experience

Professor, ERA-Chair SimEA (from July 2020 – Today)
The Cyprus Institute, CyI, Cyprus

Professor (February 2021 – Today)
Department of Mathematics and Applied Mathematics, University of Crete, Greece

Research Associate (March 2010 – Today)
Institute of Applied and Computational Mathematics (IACM), FORTH, Heraklion, Greece

Associate Professor (September 2016 – January 2021)
Department of Mathematics and Applied Mathematics, University of Crete, Greece

Visiting Scientist (January 2010 – December 2016)
Max Planck Institute for Polymer Research (MPIP), Theory Group, Mainz, Germany

Tenured Assistant Professor (December 2014 – September 2016)
Department of Applied Mathematics, University of Crete, Greece

Track Tenure Assistant Professor (September 2009 – December 2014)
Department of Applied Mathematics, University of Crete, Greece

Research Associate (October 2007 – August 2009)
Max Planck Institute for Polymer Research (MPIP), Theory Group, Mainz, Germany

Post-Doctoral Research Associate
(February 2005 – September 2007)
Max Planck Institute for Polymer Research (MPIP), Theory Group, Mainz, Germany
(May 2003 – January 2005)
Institute of Chemical Engineering and High-Temperature Chemical Processes and Department of Chemical Engineering, University of Patras, Patras, Greece

Visiting Scientist
University of Tennessee, Department of Chemical Engineering, Knoxville, USA (November 2003)

Military Service (January 2002-March 2003)
War Material Corps, Kolxiko, Salonica, and Sparti, Hellas

Ph.D. Research Assistant (September 1996-November 2001)
Department of Chemical Engineering, University of Patras, Greece, and
Institute of Chemical Engineering and High-Temperature Chemical Process (ICE/HT-FORTH)

Education

Ph.D. in Chemical Engineering
University of Patras, Greece, February 2002

- *GPA*: Highest degree
- *Dissertation*: "Atomistic Molecular Dynamics Simulations of Polymer Melt Viscoelasticity"
- *Advisor*: Prof. D.N. Theodorou

Diploma in Chemical Engineering
University of Patras, Greece, July 1996

Publications – Presentations – Other Activities (SYNOPSIS)

He has published about 80 papers in refereed journals, 4 in books, 20 in refereed conference proceedings, and about 60 in non-refereed conference proceedings. He has given more than 130 (about 80 invited) presentations in international conferences and academic and industrial institutions. As of June 30, 2021, his work has received (ISI, Web of Science) 3515 total citations (3082 non-self citations). His h-index is 31. He has been a Reviewer for a large number of International Journals, for the *European Union*, and for various institutions among which the *National Science Foundation* (USA), the *European Science Foundation*, the *Israeli Science Foundation* (ISF), *National Research Council* of Romania, and the Greek *General Secretariat for Research and Technology*. He has also been the organizer and co-organizer of about 20 International workshops and conferences.

Honors and Awards

- M.Sc. thesis "*Atomistic simulation study of star-shaped polystyrene melts*" of E. Gkolfi, supervised by V. Harmandaris, with co-supervisor P. Bačová, 1st prize for Best M.Sc. Thesis on Condensed Matter and Material Science, by the Hellenic Society for the Science and Technology of Condensed Matter, 2020.
- Who's Who in Science 2008, 2010 Edition.
- European fellowship Marie-Curie for participating in the «*International School of Solid State Physics: 34th Course: Computer Simulations in Condensed Matter*», Erice, Italy, 2005.
- Ph.D. Research assistant fellowship, Institute of Chemical Engineering and High-Temperature Chemical Process (ICE/HT-FORTH), 1996-2001.
- European fellowship for participating as a training visitor in University of Edinburgh under the program TRACS, UK, 2000.
- Outstanding Undergraduate Student Excellence Awards, 1993 and 1994.

Professional Affiliations

Member, Society of Industrial and Applied Mathematics (SIAM),

American Chemical Society (ACS),
American Physical Society (APS).
Hellenic Society of Rheology (HSR), Technical Camber of Greece (TEE).

Referee

- **Journals:** *Nature Journals* (Nature Materials, Nature Chemistry, Nature Communications), *American Chemical Society* (Macromolecules, Langmuir, Journal of the American Chemical Society, ACS Macro Letters), *American Physical Society* (Physical Review Letters, Physical Review E), Entropy, *Royal Society of Chemistry* (Soft Matter, Physical Chemistry Chemical Physics, Journal of Materials Chemistry, Nanoscale), *American Institute of Physics* (The Journal of Chemical Physics), Journal of Polymer Science Part B: Polymer Physics, Journal of Physical Chemistry, Macromolecular Theory and Simulation, Rheologica Acta, *Institute of Physics* (Journal of Physics: Condensed Matter, Journal of Physics D: Applied Physics, Modeling and Simulation in Material Science and Engineering), Journal of Non-Newtonian Fluid Mechanics, Polymer, Journal of Molecular Liquids, Molecular Simulation, Computer Physics Communications, Computational and Theoretical Chemistry, Applied Surface Science, Journal of Nanoscience and Nanotechnology, Journal of Computational Chemistry, Journal of Molecular Modeling, ISRN-Polymer Science, Composites Part A: Applied Science and Manufacturing, Journal of Adhesion, Chemical Engineering Science, European Polymer Journal, European Biophysics Journal, Chinese Journal of Chemistry, Macromolecular Symposia.
- **Review Editor** in Frontiers in Physics (Soft Matter Physics).
- **Editorial Board**: **"**Computation", MDPI; "Polymer", MDPI; "Sci", MDPI.

Reviewer for:

- European Commission.
- National Science Foundation (NSF), USA.
- ELIDEK and, General Secretariat for Research and Technology (GSRT), Greece.
- Deutschen Forschungsgemeinschaft (DFG), Germany.
- Swiss National Science Foundation (SNSF), Switzerland.
- Romanian National Research Council (Rapporteur).
- Israel National Science Foundation (INSF), Israel.
- Research Grants Council, Hong Kong.
- CECAM workshops, Europe.
- Partnership for Advanced Computing in Europe (PRACE) Expert, Europe.
- State Scholarships Foundation (IKY), Greece.
- e-COST Actions, Europe.
- High Performance Computing – ARIS proposals, GRNET, Greece.
- *Reviewer for Several International Conferences* such as: "2014 Global Conference on Polymer and Composite Materials (PCM2014)", "Advanced Computational Methods, ADVCOMP, 2015, 2016"

Organizing Conferences/Workshops

- *Chairman, or co-chairman* of about 20 national and international scientific conferences and workshops.
- *Member of Program, or Scientific, Committee* of more than 15 international scientific conferences and workshops.

Representative conferences:

1. Member of the organizing committee of the conference "10*th International Young Scientists Conference on Computational Science*", Online, YSC2021, 28 June – 2 July **2021**.
2. Member of the organizing committee of the conference "*9th International Young Scientists Conference on Computational Science*", Online, YSC2020, 05-14 September **2020**.
3. Member of the organizing committee of the conference "*8th International Young Scientists Conference on Computational Science*", Heraklion, Greece, YSC2019, 24-28 June **2019**.
4. Member of the organizing committee of the "*European Polymer Congress 2019 (EPF 2019)*", EPF 2019, Heraklion, Greece, 09-14 June **2019**.
5. Member of the organizing committee of the conference "*7th International Young Scientists Conference on Computational Science*", Heraklion, Greece, YSC2018, 02-06 July **2018**.
6. Member of the Committee for the conference "EMN 2017 Surface and Interface", Jeju, Korea, May 22-26, **2017**.
7. Member of the organizing committee of the conference "Eurofillers & Polymer Blends", Heraklion, Crete, Greece, April 23-27, **2017**.
8. Member of the organizing committee of the conference "11th Hellenic Polymer Society International Conference", Heraklion Crete, November 3-5, **2016**.
9. Member of the organizing committee of the mini-symposium "*Numerical Methods in Multi-scale Modeling of Materials*", SIAM, Philadelphia, USA, May 08-12, **2016**.
10. Organizer of the workshop "*Mathematical and Computational Techniques for Molecular Systems*", Heraklion, Greece, September 16-18, **2015**.
11. Member of the organizing committee for the symposium "*Mathematical and Computational Methods in Non-equilibrium Statistical Mechanics*", Heraklion, Greece, September 16-20, **2013**.
12. Member of the organizing committee for the workshop "*Workshop on Software Frameworks for Challenging Computational Problems*", Heraklion, Greece, January 14-18, **2013**.

Languages

Fluent in English, Greek

Computing Skills

- Excellent knowledge (system administrator during the entire Ph.D. program) of all available Unix computing systems including Linux, Silicon Graphics, IBM, Hewlett-Packard, Sun, Compaq.

- Experience in vectorization and parallelization of simulation algorithms on various machines (BlueGen, CRAY T3E, PC Linux cluster, HP9000).

News & Views

- ERCIM News 115: "Computational Design of Complex Materials Using Information Theory: from Physics to Data-driven Multi-scale Molecular Models" **V. Harmandaris**, E. Kalligiannaki, and M. Katsoulakis, October **2018**, *Special theme: Digital Twins*, https://ercim-news.ercim.eu/images/stories/EN115/EN115-web.pdf

Publications in Refereed Journals

1. W. Li, P.K. Jana, A. F. Behbahani, G. Kritikos, L. Schneider, P. Polińska, C. Burkhart, **V. Harmandaris**, M. Muller, M. Doxastakis, "Dynamics of long entangled polyisoprene melts via multiscale modeling", *Macromolecules*, **2021**, 54, 18, 8693–8713, https://doi.org/10.1021/acs.macromol.1c01376

2. P. Bačová, W. Li, , A. F. Behbahani, C. Burkhart, P. Polińska, M. Doxastakis, **V. Harmandaris**, "Coupling between polymer conformations and dynamics near rough silica surfaces: a direct insight from atomistic simulations", *Nanomaterials*, **2021**, *11*(8), 2075, https://doi.org/10.3390/nano11082075 (special issue: "*Advances in Computational Materials Science on Functional Interfaces and Surfaces*").

3. M. Arnittali, A.N. Rissanou, M. Amprazi, M. Kokkinidis, and **V. Harmandaris** "Structure and Thermal Stability of wtRop and RM6 Proteins through All-atom Molecular Dynamics Simulations and Experiments", *Int. J. of Mol. Sci.*, **2021**, 22(11), 5931. https://doi.org/10.3390/ijms22115931 (special issue: "*Folding and Design of α-Helical Proteins and Peptides: Theory Meets Nanomaterials, Biotechnology and Health*")

4. W. Li, P. Bačová, A. F. Behbahani, C. Burkhart, P. Polińska, **V. Harmandaris**, M. Doxastakis, "Tailoring interfacial properties in polymer-silica nanocomposites via surface modification: An atomistic simulation study" *ACS Appl. Mater. &Interfaces*, **2021**, *3*(5), 2576–2587, https://doi.org/10.1021/acsapm.1c00197

5. C. Alexandrou, **V. Harmandaris**, A. Irakleous, G. Koutsou, N. Savva, "Modelling the evolution of COVID-19 via compartmental and particle-based approaches: Application to the Cyprus case", PLOS One, **2021**, *16(5)*: e0250709., https://doi.org/10.1371/journal.pone.0250709

6. P. Bačová, D. Mintis, E. Gkolfi, **V. Harmandaris**, "Mikto-arm stars as soft-patchy particles: from building blocks to mesoscopic structures", *Polymers*, **2021**, *13*(7), 1114, https://doi.org/10.3390/polym13071114 (special issue: "*Self-Assembly of Block Copolymers: Experiment and Modelling of Polymers*")

7. A. F. Behbahani, **V. Harmandaris**, "Gradient of Segmental Dynamics in Stereoregular Poly(methyl methacrylate) Melts Confined Between Graphene-based Sheets" *Polymers*, **2021**, *13*, 830. https://doi.org/10.3390/polym13050830 (Special Issue "*Theory of Polymers at Interfaces*").

8. A. F. Behbahani, L. Schneider, A. Rissanou, A. Chazirakis, P. Bačová, P. Kumar Jana, W. Li, M. Doxastakis, P. Polińska, C. Burkhart, M. Muller, and **V. Harmandaris**, "Dynamics and Rheology of Polymer Melts via Hierarchical Atomistic, Coarse-grained, and Slip-spring Simulations" *Macromolecules*, **2021**, *54*, 6, 2740–2762, http://dx.doi.org/10.1021/acs.macromol.0c02583 (*Chosen as back-cover*).

9. D. Stefanakis, **V. Harmandaris**, G. Kopidakis, and I. Remediakis, "From order to disorder of alkanethiol SAMs on complex Au (211), (221) and (311) surfaces: Impact of the substrate", *J. Phys. Chem. C*, **2021**, *125*, 6, 3495–3508, https://doi.org/10.1021/acs.jpcc.0c08328

10. A. Power, I. Remediakis and **V. Harmandaris**, "Interface and Interphase in Polymer Nanocomposites with Bare and Core-Shell Gold Nanoparticles", *Polymers*, **2021**, *13*(4), 541, 1-28, https://doi.org/10.3390/polym13040541 (Special Issue "*Modeling and Simulation of Polymer Nanocomposites*").

11. P. Bačová, E. Glynos, S. Anastasiadis and **V. Harmandaris**, "How does the number of arms affect the properties of mikto-arm stars in a selective oligomeric matrix? Insights from atomistic simulations", *ACS Omega*, **2021**, *6*, 1138−1148, https://doi.org/10.1021/acsomega.0c04167

12. E. Gkolfi, P. Bačová, and **V. Harmandaris**, "Size and shape characteristics of polystyrene and poly(ethylene oxide) star-shaped melts studied by atomistic simulations", *Macrom. Theor. Simul.*, **2021**, *30*(1), 2000067, https://doi.org/10.1002/mats.202000067 (*Chosen as front-cover*).

13. P. Bačová, E. Gkolfi, L. Hawke and **V. Harmandaris**, "Dynamical heterogeneities in non-entangled polystyrene and poly(ethylene oxide) star melts", *Phys. of Fluids*, **2020**, *32*, 127117, https://doi.org/10.1063/5.0031856

14. A. Rissanou, A. Keliri, M. Arnittali and **V. Harmandaris**, "Self-Assembly of Diphenylalanine Peptides on Graphene via Detailed Atomistic Simulations", *Phys. Chem. Chem. Phys.*, **2020**, *22*, 27645-27657, https://doi.org/10.1039/D0CP03671D.

15. T. Jin, A. Chazirakis, E. Kalligiannaki, **V. Harmandaris**, M. Katsoulakis, "Data-driven uncertainty quantification for systematic coarse-grained models" Soft Materials, **2020**, *18:2-3*, 348-368, https://doi.org/10.1080/1539445X.2020.1765803

16. A. Rissanou, G. Simatos, P. Siachouli, **V. Harmandaris** and A. Mitraki, "Self-assembly of alanine-isoleucine and isoleucine-isoleucine dipeptides through atomistic simulations and experiments", *J. Phys. Chem. B*, **2020**, 124, 33, 7102–7114, https://doi.org/10.1021/acs.jpcb.0c03025. (*Chosen as back-cover*).

17. G. Kritikos, A. Rissanou, **V. Harmandaris** and K. Karatasos, "Bound layer polymer behavior on graphene and graphene oxide nanosheets", *Macromolecules*, **2020**, *53*, 15, 6190–6203, https://dx.doi.org/10.1021/acs.macromol.0c01040

18. A. F. Behbahani, A. Rissanou, G. Kritikos, M. Doxastakis, C. Burkhart, P. Polińska and **V. Harmandaris**, "Conformations and dynamics of polymer chains in cis and trans Poly(butadiene)/Silica nanocomposites through atomistic simulations: From the un-entangled to the entangled regime", *Macromolecules*, **2020**, *53*, 15, 6173–6189, https://dx.doi.org/10.1021/acs.macromol.0c01030.

19. W. Lei, C. Burkhart, P. Polińska, **V. Harmandaris** and M. Doxastakis, "Backmapping coarse-grained macromolecules: an efficient and versatile machine-learning approach", *J. Chem. Phys*, **2020**, *153*, 041101, https://doi.org/10.1063/5.0012320.

20. P. Bačová, E. Glynos, S. Anastasiadis and **V. Harmandaris**, "Spatio-temporal heterogeneities in nanosegregated single-molecule polymeric nanoparticles", *Soft Matter*, **2020**, *16*, 4584, https://doi.org/10.1039/d0sm00079e. (*Chosen as back-cover*).

21. N. Shahidi, A. Chazirakis, **V. Harmandaris** and M. Doxastakis, "Coarse-graining of polyisoprene melts using inverse Monte Carlo and local density Potentials", *J. Chem. Phys.*, **2020**, *152*, 124902, https://doi.org/10.1063/1.5143245.

22. A. Rissanou, P. Bačová, **V. Harmandaris**, "Properties of nanographene in polymer nanocomposites through all-atom simulations: Shape fluctuations and rippling", Comp. Mat. Sc, **2020**, *172*, 109330, https://doi.org/10.1016/j.commatsci.2019.109330

23. A. Rissanou, P. Bačová, **V. Harmandaris**, "Investigation of the properties of nanographene in polymer nanocomposites through molecular simulations: Dynamics and anisotropic Brownian motion", PCCP, **2019**, *21*, 23843-23854, https://doi.org/10.1039/c9cp02074h (*Chosen as back-cover*).

24. A. F. Behbahani, S.M. Vaez Allaei, G.H. Motlagh, H. Eslami and **V. Harmandaris**, "Structure and conformation of stereoregular poly(methyl methacrylate) chains adsorbed on graphene oxide and reduced graphene oxide via atomistic simulations", *Macromolecules*, **2019**, *52*, 3825−3838, https://doi.org/10.1021/acs.macromol.9b00574

25. P. Bačová, E. Glynos, S. Anastasiadis and **V. Harmandaris**, "Nanostructuring single-molecule polymeric nanoparticles via macromolecular architecture host", *ACS Nano*, **2019**, *13*, 2, 2439-2449, https://doi.org/10.1021/acsnano.8b09374.

26. G. Zhang, A. Chazirakis, **V. Harmandaris**, T. Stuehn, K. Daoulas, and K. Kremer, "Hierarchical modelling of polystyrene melts: from soft blobs to atomistic resolution", *Soft Matter*, **2019**, *15*, 289-302, https://doi.org/10.1039/c8sm01830h.

27. P. Bačová, R. Foskinis, E. Glynos, A. Rissanou, S. Anastasiadis and **V. Harmandaris**, "Effect of macromolecular architecture on the self-assembly behavior of copolymers in a selective polymer host", *Soft Matter*, **2018**, 14, 9562-9570, https://doi.org/10.1039/c8sm01421c (*Chosen as back-cover*).

28. A. F. Behbahani, S.M. Vaez Allaei, G.H. Motlagh, H. Eslami and **V. Harmandaris**, "Structure, dynamics, and apparent glass transition of stereoregular poly(methyl methacrylate)/graphene interfaces through atomistic simulations", *Macromolecules*, **2018**, *51*, 7518-7532, doi: acs.macromol.8b01160. http://dx.doi.org/10.1021/acs.macromol.8b01160

29. A. F. Behbahani, S.M. Vaez Allaei, G.H. Motlagh, H. Eslami and **V. Harmandaris**, "Structure and dynamics of stereo-regular poly(methyl-methacrylate) melts through atomistic molecular dynamics simulations", *Soft Matter*, **2018**, *14*, 1449-1464. https://doi.org/10.1039/C7SM02008B

30. A. Tsourtis, **V. Harmandaris**, D. Tsagkarogiannis, "Parameterization of coarse-grained molecular interactions through potential of mean force calculations and cluster expansions Techniques", *Entropy*, **2017**, *19*, 395, https://doi.org/10.3390/e19080395

31. A. Rissanou, H. Papananou, V. Petrakis, M. Doxastakis, K. Andrikopoulos, G. Voyiatzis, K. Chrissopoulou, **V. Harmandaris**, S. Anastasiadis, "Structural and conformational properties of poly(ethylene oxide)/silica nanocomposites: Effect of confinement", *Macromolecules*, **2017**, *50*, 6273-6284, http://dx.doi.org/10.1021/acs.macromol.7b00811

32. M. Gulde, A. Rissanou, **V. Harmandaris**, M. Müller, S. Schäfer, C. Ropers "Structure and dynamics of monolayer polymer crystallites on graphene", *Nano Letters*, **2016**, *16*, 6994–7000; http://dx.doi.org/10.1021/acs.nanolett.6b03079

33. E. Kalligiannaki, A. Chazirakis, A. Tsourtis, M. Katsoulakis, P. Plechac, **V. Harmandaris**, "Parametrizing coarse grained models for molecular systems at equilibrium", *Europ. Phys. J. Special Topics*, **2016**, *225*, 1347–1372. doi: http://dx.doi.org/10.1140/epjst/e2016-60145-x

34. **V. Harmandaris**, E. Kalligiannaki, M. Katsoulakis, P. Plechac, "Path-space variational inference for non-equilibrium coarse-grained systems", *J. Comp. Phys.*, **2016**, *314*, 355–383. Doi:10.1016/j.jcp.2016.03.021 https://doi.org/10.1016/j.jcp.2016.03.021

35. P. Bačová, A. Rissanou, **V. Harmandaris**, "Edge-functionalized graphene as a nanofiller: Molecular dynamics simulation study", *Macromolecules*, **2015**, *48*, 9024–9038, http://pubs.acs.org/doi/10.1021/acs.macromol.5b01782.

36. E. Kalligiannaki, **V. Harmandaris**, M. Katsoulakis, P. Plechac "The geometry of generalized force matching and related information metrics in coarse-graining of molecular systems", *J. Chem. Phys.*, **2015**, *143*, 084105. http://dx.doi.org/10.1063/1.4928857

37. A. Tsourtis, Y. Pantazis, M. Katsoulakis, **V. Harmandaris**, "Parametric sensitivity analysis for stochastic molecular systems using information theoretic metrics", *J. Chem. Phys.*, **2015**, *143*, 014116. https://doi.org/10.1063/1.4922924

38. A. Rissanou, **V. Harmandaris**, "Structural and dynamical properties of polystyrene thin films", *Macromolecules*, **2015**, *48*, 2761–2772, https://doi.org/10.1021/ma502524e

39. A. Rissanou, A. Power, **V. Harmandaris**, "Properties of polyethylene/graphene nanocomposites through molecular dynamics simulations", *Polymers*, **2015**, *7*, 390-417, https://doi.org/10.3390/polym7030390

40. H. J. Butt, H. Duran, W. Egger, F. Faupel, **V. Harmandaris**, S. Harms, K. Johnston, K. Kremer, Y. Lin, L. Lue, C. Ohrt, K. Raetzke, L. Ravelli, W. Steffen, and S. D. B. Vianna, "Interphase of a polymer at a solid interface", *Macromolecules*, **2014,** *47*, 8459-8465, https://doi.org/10.1021/ma501747j

41. **V. Harmandaris**, "Quantitative study of equilibrium and non-equilibrium polymer dynamics through systematic hierarchical coarse-graining simulations", *Korea-Aust. Rheol. J.*, **2014**, *26*, 15-28. https://doi.org/10.1007/s13367-014-0003-7

42. A. Rissanou, **V. Harmandaris**, "Dynamics of various polymer/graphene interfacial systems through atomistic molecular dynamics simulations", *Soft Matter*, **2014**, *10*, 2876-2888.

43. K. Johnston, **V. Harmandaris**, "Hierarchical multiscale modeling of polymer−solid interfaces: Atomistic to

coarse-grained description and structural and conformational properties of polystyrene−gold systems", *Macromolecules*, **2013,** *46*, 5741−5750; https://doi.org/10.1021/ma400357r

44. **V. Harmandaris**, M. Doxastakis "Molecular dynamics of polyisoprene/polystyrene oligomer blends: The role of self-concentration and fluctuations on blend dynamics", *J. Chem. Phys.*, **2013,** *139*, 034904, https://doi.org/10.1063/1.4813019

45. A. Rissanou, **V. Harmandaris**, "A molecular dynamics study of polymer/graphene nanocomposites", *Macromolecular Symposia*, **2013**, *331-332*, 43–49, https://doi.org/10.1002/masy.201300070

46. K. Johnston, **V. Harmandaris**, "Hierarchical simulations of hybrid polymer/solid materials", *Soft Matter*, **2013**, *9*, 6696-6710 (Review article, Themed Issue on Emerging Investigators). https://doi.org/10.1039/C3SM50330E

47. **V. Harmandaris**, G. Floudas, K. Kremer, "Dynamic heterogeneity in fully miscible blends of polystyrene with oligostyrene", *Phys. Rev. Let.* **2013**, *110*, 165701; https://doi.org/10.1103/PhysRevLett.110.165701

48. A. Rissanou, **V. Harmandaris**, "Structure and dynamics of poly(methyl-methacrylate)/graphene systems through Atomistic molecular dynamics Simulations", *Journal of Nanoparticle Research* **2013**, 15, 1589, https://doi.org/10.1007/s11051-013-1589-2

49. A. Rissanou, E. Georgilis, M. Kasotaskis, A. Mitraki, **V.A. Harmandaris**, "Effect of solvent on the self-assembly of dialanine and diphenylalanine peptides", *J. Phys. Chem. B* **2013**, *117*, 3962-3975, https://doi.org/10.1021/jp311795b

50. K. Johnston, **V. Harmandaris**, "Properties of short polystyrene chains confined between two gold surfaces through a combined density functional theory and classical molecular dynamics approach", *Soft Matter*, **2012,** *8*, 6320-6332, https://doi.org/10.1039/C2SM25567G

51. K. Johnston, **V. Harmandaris**, "Properties of benzene confined between two Au(111) surfaces using a combined density functional theory and classical molecular dynamics approach", *J. Phys. Chem. C* **2011**, *115*, 14707-14717, https://doi.org/10.1021/jp2003485

52. D. Fritz, K. Koschke, **V. Harmandaris**, N.F.A. van der Vegt and K. Kremer, "Multiscale modeling of soft matter: scaling of dynamics", *Phys. Chem. Chem. Phys.*, **2011**, *13*, 10412-10420, https://doi.org/10.1039/C1CP20247B

53. **V. Harmandaris**, G. Floudas, K. Kremer, "Temperature and pressure dependence of polystyrene dynamics through molecular dynamics simulations and experiments", *Macromolecules* **2011**, *44*, 393-402, https://doi.org/10.1021/ma102179b

54. C. Baig, **V. Harmandaris** "Quantitative Analysis on the Validity of a Coarse-Grained Model for Nonequilibrium Polymeric Liquids under Flow", *Macromolecules*, **2010**, *43*, 3156-3160, https://doi.org/10.1021/ma100070p

55. D. Fritz, **V. Harmandaris**, K. Kremer, N. van der Vegt, "Coarse-Grained polymer melts based on isolated atomistic chains: Simulation of polystyrene of different tacticities", *Macromolecules*, **2009**, *42*, 7579-7588, https://doi.org/10.1021/ma901242h

56. **V. Harmandaris**, K. Kremer, "Predicting polymer dynamics at multiple length and time scales", *Soft Matter*, **2009**, *5*, 3920-3926, https://doi.org/10.1039/B905361A

57. T. Cherdhirankorn, **V. Harmandaris**, A. Juhari, P. Voudouris, G. Fytas, K. Kremer, K. Koynov, "Fluorescence correlation spectroscopy study of molecular probe diffusion in polymer melts", *Macromolecules* **2009**, *42*, 4858-4866, https://doi.org/10.1021/ma900605z

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68. **V. Harmandaris,** V.G. Mavrantzas, D.N Theodorou, "From chemical structure to polymer processing: Atomistic simulation of the viscoelasticity of linear polyethylene melts", Proceedings*, 4th Panhellenic Conference on Polymers*, Patras, Greece, November 20-22, **1997**.

Invited Presentations

1. **V. Harmandaris,** "Mechanical and Viscoelastic Properties of Polymer Nanocomposites: The role of Interphases", *13th Hellenic Polymer Society International Conference*, Athens, 27-29 December **2021.**
2. **V. Harmandaris,** "Polymer Melts and Polymer Nanocomposites via Simulations across Scales: from Atoms to Macroscopic Properties", *European Polymer Conference, EPF 2022 – Inter Congress Workshop* (On-line), 28 June **2021**.
3. **V. Harmandaris,** " Characterization of Liquid/Solid Interfaces via Hierarchical Simulations Across Scales: A synergy between Simulations and Data-driven Algorithms", *EMLG/JMLG Workshop*, Cyberspace, 13 September **2021.**
4. **V. Harmandaris,** " Computational Modeling of Soft Matter Across Scales: From Atoms to the Design of Materials", (Invited Lecture) Computational modeling of polymer-based nanostructured materials: A synergy between simulations and data-driven algorithms", *16th International Summer Schools on Nanosciences & Nanotechnologies, Organic Electronics and Nanomedicine (ISSON21)*, Thessaloniki, Greece, 3-10 July **2021.**
5. **V. Harmandaris,** "Computational modeling of polymer-based nanostructured materials: A synergy between simulations and data-driven algorithms", *18th International Conference on Nanosciences & Nanotechnologies (NN21)*, Thessaloniki, Greece, 6-9 July **2021.**
6. **V. Harmandaris,** "Hierarchical Coarse-Graining of Molecular Systems: Physics-based vs Data-driven Models and Uncertainty Quantification", *4th International Conference on Uncertainty Quantification in Computational Sciences and Engineering Science,* Cyberspace, 28-30 June **2021.**

7. **V. Harmandaris,** " Computational Modelling of Soft Matter Across Scales: From Atoms to Macroscopic Properties of Materials", *Colloquium, Statistical Physics Group, Coventry University*, 2 June **2021.**
8. **V. Harmandaris,** "Hierarchical Coarse-Graining of Macromolecules: Physics-based or Data-driven Models?" *SIAM Conference on Mathematical Aspects of Materials Science – MS 21*, Cyberspace May 17-28, **2021.**
9. **V. Harmandaris,** "Simulations of Polymer-based Materials Across Length and Time Scales", *Workshop on "Computational Materials Science"*, Department of Materials, University of Crete, December 20, **2020.**
10. **V. Harmandaris,** " Molecular Simulations of Polymeric Nanostructured Materials across Length and Time Scales", *Colloquium, Physics department, University of Ioannina*, October 23, **2020.**
11. **V. Harmandaris,** " Multi-scale Simulation Study of Polymer Nanocomposites via Hybrid Physics-based Data-driven Models", *2nd BGU-FORTH/UoC Soft Matter workshop on Bio-and-synthetic nanostructures, polymers, colloids, and gels*", Beer Sheva, Ben Gurion Univ., Israel, 25-27 February **2020.**
12. **V. Harmandaris**, "Hierarchical Multi-scale Modeling of Molecular Systems: Current Trends and Challenges", *CIB-CECAM,* EPFL, Switzerland, 20-30 May **2019.**
13. **V. Harmandaris**, "Molecular Simulations of Polymeric Nanostructured Materials", *12th Hellenic Polymer Society International Conference,* Ioannina, Cyprus, September 30 – October 03, **2018.**
14. **V. Harmandaris**, "Molecular Simulations of Polymer-based Nanostructured Materials", *ICPAM 12,* Heraklion, Crete, September 22-28, **2018.**
15. **V. Harmandaris**, "Molecular Simulations of Complex Polymeric Nanostructured Materials", *XXXIII Panhellenic Conference on Solid State Physics and Materials Science,* Nicosia, Cyprus, September 17-19, **2018.**
16. **V. Harmandaris**, "Hierarchical Multiscale Simulations of Complex Nanostructured Materials", *Symposium on Model, Algorithms and Data,* FORTH/IACM, Crete, July 17-18, **2018.**
17. **V. Harmandaris**, "Hierarchical Multiscale Simulations of Polymeric Nanostructured Materials", *ETH,* Polymer Physics, Zurich, Swiss, Greece, April 11, **2018.**
18. **V. Harmandaris**, "Mathematical and Computational Modeling of Molecular Systems", *11th FORTH Retreat*, Crete, Greece, 13th October, **2017.**
19. **V. Harmandaris**, "Hierarchical Multiscale Modeling of Molecular Systems: From Molecular to Stochastic Dynamics", *International Conference on Scientific Computation and Differential Equations (SciCADE),* Invited in the mini-s*ymposium*: Molecular Dynamics, Bath, UK, 11-15th September, **2017.**
20. **V. Harmandaris**, "Properties of Graphene/Polymer Nanostructured Systems through Atomistic Simulations", *10th International Symposium on Flexible Organic Electronics (ISFOE17),* Thessaloniki, Greece, 3-6 July, **2017.**
21. **V. Harmandaris**, "Hierarchical Multiscale Modeling of Molecular Systems: From Atomistic to Coarse-Grained Description", *Colloquium, Department of Mathematics and Statistics*, University of Sussex, UK, 22th June, **2017.**
22. **V. Harmandaris**, "Molecular Simulations of Graphene based Polymer Nanostructured Materials", *Colloquium, Department of Materials*, University of Crete, Greece, 14th November, **2016.**
23. **V. Harmandaris**, "Mathematical and Computational Modeling of Complex Molecular Systems", *2nd Hellenic Workshop on 2D Materials,* Heraklion, Crete, Greece, 01-02nd November, **2016.**
24. **V. Harmandaris**, "Structure and dynamics of polymer/nano-graphene nanocomposites through molecular simulations", *2nd Israel-Greece Joint Meeting on Nanotechnology and BioNanoscience,* Heraklion, Crete, Greece, 25-28th October, **2016.**
25. **V. Harmandaris**, "Hierarchical Multiscale Modeling of Nanostructured Polymeric Materials: II) Mesoscopic (Coarse-grained) Simulations", Workshop on *Simulation of Protein Interactions with Surfaces and Nanoparticles*, Institute for Research in fundamental Sciences (IPM), School of Nano Science, Tehran, Iran, 19-20th October, **2016.**
26. **V. Harmandaris**, "Hierarchical Multiscale Modeling of Nanostructured Polymeric Materials: I) Microscopic (Quantum and Classical) Simulations", Workshop on *Simulation of Protein Interactions with Surfaces and Nanoparticles*, Institute for Research in fundamental Sciences (IPM), School of Nano Science, Tehran, Iran, 19-20th October, **2016**
27. **V. Harmandaris**, "Hierarchical Multiscale Modelling of Hybrid Nanostructured Polymeric Materials", *Soft Matter Meeting Israel – Greece FORTH-BGU workshop on polymers, colloids, gels, bio-and-synthetic nanostructures*, Heraklion, Crete, Greece, 25-27th September, **2016.**

28. **V. Harmandaris**, "From Atomistic to Systematic Coarse-Grained Models for Molecular Systems", *SIAM Conference on Mathematical Aspects of Materials Science MS: Numerical Methods in Multiscale Materials Modelling*, Philadelphia, 07-12th May, **2016.**
29. **V. Harmandaris**, "Hierarchical Multi-scale Modeling of Polymers and Interfaces", *Second CCPBioSim/CCP5 Multiscale Modelling Conference*, University of Manchester, UK, April 13-15, **2016.**
30. **V. Harmandaris**, "Hierarchical Multi-scale Modeling of Hybrid Polymer/Solid Nanostructured Systems", *Webinar Computational Mathematics Pacific Northwest National Laboratory (PNNL),* September 28, **2015**.
31. **V. Harmandaris**, "Mathematical and Computational Modeling of Materials" (in Greek), *Workshop on Novel Materials for New Technologies*, Department of Materials, University of Crete, Greece, September 28, **2015**.
32. **V. Harmandaris**, A. Rissanou, D. Tzeli, "Self-assembly of Diphenylalanine and Chemically Modified Diphenylalanine Peptides on Various Solvents", *Workshop on Self-Assembly in Soft Matter*, University of Patras, Greece, September 01–02, **2015.**
33. **V. Harmandaris**, "Dynamics of Graphene based Polymer Nanocomposites through Molecular Simulations", *Rheology Symposium in honor of Prof. Roger I. Tanner,* Samos, Greece, June 29 – July 03, **2015**.
34. **V. Harmandaris**, "Detailed molecular simulations of grapheme based polymer nanocomposites", *Workshop on Polymer Nanocomposites*, National Technical University of Athens, Greece, June 16-17, **2015**.
35. **V. Harmandaris**, "Hierarchical Modeling of Hybrid Polymer/Solid Nanostructured Systems", *Mainz Materials Simulation Days: Non-Equilibrium Processes in Soft Matter*, Mainz, Germany, June 10-13, **2015**.
36. **V. Harmandaris**, "Systematic Hierarchical Simulations of Hybrid Polymer/Solid Systems", *CECAM Meeting: MD Meets Fluctuating Hydrodynamics,* Madrid, Spain, May 10-13, **2015**.
37. **V. Harmandaris**, P. Bačová, A. Rissanou, "Study of Hybrid Polymer/Solid and Graphene based Polymer Nanocomposites through Molecular Simulations", *COST Action MP1202 HINT: Annual Meeting*, Heraklion, Crete, April 20-23, **2015**.
38. **V. Harmandaris**, "Hierarchical Multi-scale Modeling of Polymer Nanocomposites", *Department of Mathematics and Statistics, University of Cyprus,* Cyprus, December 19, **2014**.
39. **V. Harmandaris**, "Hierarchical Multi-scale Modeling of Hybrid Polymer/Graphene Systems", *Department of Physics, University of Goettingen,* Goettingen, Germany November 04, **2014**.
40. **V. Harmandaris**, "Hierarchical Multi-scale Modeling of Hybrid Polymer/Solid Complex Systems", *Multiscale Computational Methods in Materials Modelling*, Edinburgh, UK, June 17-21, **2014**.
41. **V. Harmandaris**, "Simulations of Soft Matter under Equilibrium and Non-equilibrium Conditions", *International Conference on Applied Mathematics*, ACMAC Center, Heraklion, Greece, September 16, **2013**.
42. **V. Harmandaris**, "Modeling of hybrid polymer/solid interfacial systems", *246th ACS National Meeting & Exposition*, Indianapolis, USA, September 09, **2013**.
43. **V. Harmandaris**, "Studying Soft Matter through Hierarchical Multi-scale Modeling", *CCP5 Summer School, Methods in Molecular Simulations*, University of Manchester, UK, July 29, **2013.**
44. **V. Harmandaris**, "Hierarchical Multi-scale Simulations of Polymer/Metal Interfaces", *7th International Discussion Meeting on Relaxations in Complex Systems*, Barcelona, Spain, July 22, **2013.**
45. **V. Harmandaris**, "Studying soft condensed matter physics through hierarchical multi-scale modeling", *Colloquium, Department of Physics*, University of Crete, Greece, March 28, **2013.**
46. **V. Harmandaris**, "Molecular Simulations of Biomolecular Systems", *ACMAC workshop on "Cell biology and physiology: PDE models"*, ACMAC Center, Heraklion, Crete, Greece, October 4-6, **2012**.
47. **V. Harmandaris**, "Multi-scale modelling of hybrid molecule/metal nanostructures", *Workshop on "Metal nanoparticles for advanced materials: from theory to practice"*, University of Crete, Heraklion, Greece, October 1-3, **2012**.
48. **V. Harmandaris**, "Hierarchical modeling of polymer nanocomposites: From ab-initio, to atomistic up to coarse-grained simulations", *KITP Research Program,* Santa Barbara, USA, June 10-20, **2012**.
49. **V. Harmandaris**, "Hierarchical modeling of polymer nanocomposites: From ab-initio, to atomistic up to coarse-grained simulations", *Colloquium, Department of Materials*, University of Crete, Greece, May 11, **2012**.

50. **V. Harmandaris**, "Multi-scale molecular simulations of polymer interfaces", *IMPRS Workshop on "Characterization of polymer interfaces/surfaces/thin films"*, Wittenberg, Germany, April 23-27, **2012**.
51. **V. Harmandaris**, "Hierarchical multi-scale modeling of polymers under equilibrium and non-equilibrium conditions: Computational and mathematical aspects", *Workshop on "Coarse–graining of many–body systems: analysis, computations and applications"*, Heraklion, Crete, June 27 – July 1, **2011**.
52. **V. Harmandaris**, "Multiscale modeling of polymers under equilibrium and non-equilibrium conditions" *CECAM/ACAM Workshop on Dynamic Coarse-Graining: Towards quantitative mesoscale modeling of complex fluids,* Ireland, May 18-21, **2010**.
53. **V. Harmandaris**, "Hierarchical multi-scale modeling of soft matter", *Colloquium, Department of Materials*, University of Crete, Greece, May 14, **2010**.
54. **V. Harmandaris**, "Molecular friction in polymers studied by multiscale simulations", *CECAM/ACAM Workshop on Molecular Friction, Dublin,* Ireland, December 14-16, **2009**.
55. **V. Harmandaris**, "Quantitative predictions of polymer dynamics at multiple length and time scales", *Mainz Simulation Days, Mainz,* Germany, June 3-5, **2009**.
56. **V. Harmandaris** "Modeling of polymers: Methods and applications", *Max Planck Institute for Mathematics in the Sciences*, Leipzig, Germany, March 17, **2008**.
57. **V. Harmandaris**, "Multi-scale dynamic modeling of polymer and biopolymers", *Université Catholique de Louvain , Louvain-la-Neuve,* Belgium, October 12-14, **2008**.
58. **V. Harmandaris** "Structure and dynamics of polymers through hierarchical dynamic simulations", *XXIV Panhellenic Conference on Solid State Physics and Materials Science*, Heraklion, Greece, September 21-24, **2008**.
59. **V. Harmandaris** "Dynamics of polymer melts in polymer/solid interfacial systems", DECHEMA, Frankfurt, Germany, June 13, **2008**.
60. **V. Harmandaris** "Computational multiscale modeling of polymers: Methods and applications", *Workshop on Efficiency in and Modeling with Computational SPDE's*, Bonn, Germany, April 3-5 **2008**.
61. **V. Harmandaris** "Hierarchical modeling of polymer and biopolymers", *Eindhoven University of Technology, Department of Applied Physics*, Holland, November 06, **2007**.
62. **V. Harmandaris** "Coarse graining simulations of polymers: II) Dynamics and biological applications", *Workshop on Mathematical and Computational Methods for Accelerated Molecular, Stochastic and Hybrid Simulation*, Heraklion, Crete, Greece, June 25-27, **2007**.
63. **V. Harmandaris** "Coarse graining simulations of polymers: I) Methods and applications", *Workshop on Mathematical and Computational Methods for Accelerated Molecular, Stochastic and Hybrid Simulation*, Heraklion, Creta, Greece, June 25-27, **2007**.
64. **V. Harmandaris** "Mesoscopic simulations of polymers and biopolymers", *Institute of Solid State Research (IFF), Theoretical Soft-Matter and Biophysics*, Jülich, Germany, February 21, **2006**.
65. **V. Harmandaris** "Polymer dynamics at interfaces: what atomistic simulations can tell us", *Jülich Soft Matter Days 2005*, Bonn, Germany, November 01-04, **2005.**
66. **V. Harmandaris** "Atomistic modelling of polymer/solid interfaces", Department of Chemical Engineering, University of Twente, Holland, April **2004**.
67. **V. Harmandaris** "Atomistic simulation of the viscoelasticity of polymer melts: From Rouse to reptation theory", Department of Chemical Engineering, University of Tennessee, Knoxville, USA, November **2003**.
68. **V. Harmandaris** "Extracting linear viscoelastic properties from chemical constitution via atomistic molecular dynamics simulations", Max-Planck Institute for Polymer Research (MPI-P), Mainz, Germany, October **1999**.

Presentations

69. **V. Harmandaris,** " Mechanical Properties of Glassy Polymer Nanocomposites via Simulations Across Scales: The Role of Interphases", *XXV Panhellenic Conference on Solid State Physics and Materials*, Cyberspace, 27-29 September **2021.**
70. **V. Harmandaris**, "Dynamics and Rheology of Polymer Melts and Polymer Nanocomposites via Simulations Across Multiple Scales", *AERC 2021 - The Annual European Rheology Conference*, Cyberspace, April 13-15, **2021**.
71. **V. Harmandaris**, "Multi-scale Simulations of Polymer Nanocomposites with Inorganic or Polymer-based

Nanoparticles", *ICR 2020 - 18th International Congress on Rheology,* Virtual format, 14-17 December, **2020**.

72. **V. Harmandaris**, "Systematic Coarse-Grained Models for Molecular Systems Using Entropy", *5th International Conference on Entropy and its Applications*, November 18-30, **2019**.
73. **V. Harmandaris**, "Molecular Simulations of Graphene-based Polymeric Nanostructured Materials", *8th International Meeting of the Hellenic Society of Rheology*, Limassol, Cyprus, July 12-14, **2017**.
74. **V. Harmandaris**, "Molecular Simulations of Graphene-based Polymeric Nanostructured Materials", 11th *Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 25–27, **2017**.
75. **V. Harmandaris**, "Atomistic Molecular Dynamics Simulations of Multi-phase Polymer/Graphene Nanostructured Systems", 11th *Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 25–27, **2017**.
76. **V. Harmandaris**, "Properties of Nanographene Sheets in Polymer/Graphene Nanocomposites", 11th *Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 25–27, **2017**.
77. **V. Harmandaris**, "Dynamics of Graphene based Polymer Nanostructured Materials through Molecular Simulations", 10th *Panhellenic Chemical Engineers' Conference*, Patras, Greece, June 04–06, **2015**.
78. **V. Harmandaris**, "Dynamic Heterogeneity in Fully Miscible Polymer Blends through Molecular Simulations", *10th Hellenic Polymer Society Conference,* Patras, Greece, December 04-06, **2014**.
79. **V. Harmandaris**, "Study of Polystyrene Melts through Atomistic and Coarse-grained Models", *7th International Meeting of the Hellenic Rheology Society,* Heraklion, Greece, July 07-10, **2014**.
80. **V. Harmandaris**, "Molecular Dynamics Study of Graphene based Polymer Nanocomposites", *16th European Conference on Composite Materials, ECCM*, Seville, Spain, June 21-27, **2014**.
81. **V. Harmandaris**, "Studying Miscible Polymer Blends through Molecular Simulations", *Soft Comp Annual Meeting,* Heraklion, Greece, May 25-29, **2014**.
82. **V. Harmandaris**, "Hierarchical Modeling of Polymer/Solid Interfaces: From Ab-initio Calculations to Atomistic up to Coarse-grained Simulations", *APS March Meeting*, Denver, Colorado, USA, March 03-07, **2014**.
83. **V. Harmandaris**, "Polymer/graphene systems through atomistic simulations", *9th Hellenic Polymer Society Conference"*, Salonika, Greece, November 29 – December 1, **2012**.
84. K. Johnston, **V. Harmandaris**, "Multi-scale modeling of polystyrene between gold surfaces", *9th Hellenic Polymer Society Conference"*, (Poster) Salonika, Greece, November 29 – December 1, **2012**.
85. **V. Harmandaris**, "Hierarchical modeling of polymers under non-equilibrium conditions: from atomistic to coarse-grained models", *XVIth International Congress on Rheology*, Lisbon, Portugal, August 5-10, **2012**.
86. **V. Harmandaris**, "Hierarchical modeling of polymer/solid interfacial systems: From ab-initio, to atomistic up to coarse-grained simulations", Proceedings, *XI International Conference on Nanostructured Materials,* Rhodes, Greece, August, 26-31, **2012**.
87. **V. Harmandaris**, "Properties of polystyrene/graphene systems through detailed atomistic simulations", *Soft Comp Annual Meeting,* Heraklion, Greece, May 10-13, **2012**.
88. **V. Harmandaris**, "Multi-scale simulations of fluid/solid hybrid composite systems", *18th International Conference on composite materials,* Busan, Jeju Island, Korea, August, 20-26, **2011**.
89. **V. Harmandaris**, "A novel method for measuring the bending and the Gaussian rigidity of multi-component membranes by simulating tethers", *International Soft Matter Conference 2010, ISMC*, Granada, Spain, July 04-08, **2010**.
90. **V. Harmandaris**, "Multiscale modeling of polymers under equilibrium and non-equilibrium conditions: from atomistic to coarse-grained models", *International Soft Matter Conference 2010, ISMC*, Granada, Spain, July 04-08, **2010**.
91. **V. Harmandaris**, "Polymer/solid interfaces through multi-scale simulations", *17th Conference on Composite Materials, ICCM*, Edinburgh, Scotland, July 27-31, **2009**.
92. **V. Harmandaris**, "Dynamics of entangled polystyrene through hierarchical multi-scale simulations", *7th Hellenic Polymer Conference*, Ioannina, Greece, September 28-Octomber 01, **2008**.
93. **V. Harmandaris,** N.F.A. van der Vegt, K. Kremer "Dynamics of polymers through hierarchical dynamic simulations", *International Workshop on Molecular Modeling and Simulation in Applied Material Science*, DECHEMA, Frankfurt, Germany, March 10-11, **2008.**
94. **V. Harmandaris,** N.F.A. van der Vegt, K. Kremer "Comparing CG models: polystyrene", (Poster)

International Soft Matter Days, Aachen, Germany, October 1-4, **2007.**

95. **V. Harmandaris,** M. Deserno, "Studying the curvature elasticity of biomembranes through numerical simulations", (Poster) *International Soft Matter Days*, Aachen, Germany, October 1-4, **2007.**
96. **V. Harmandaris,** N.F.A. van der Vegt, K. Kremer "Structural and dynamical properties of Polystyrene determined by coarse-graining MD Simulations", (Poster) *International Discussion Meeting on the Molecular and Structural Basis of Functional Systems,* Mainz, Germany, September 26 –28, **2007.**
97. **V. Harmandaris,** M. Deserno, "Curvature elasticity of tethers", *Meeting of the German Physical Society (DPG) 2007*, Dresden, Germany, March 27 – 31, **2007.**
98. **V. Harmandaris,** M. Deserno. "A novel method for measuring the bending rigidity of model lipid membranes by simulating tethers", (Poster) *4th International Workshop on non-Equilibrium Thermodynamics and Complex Fluids, Rhodes*, Greece, September 3-7, **2006.**
99. **V. Harmandaris,** M. Deserno, "Studying the curvature elasticity of biomembranes through numerical simulations", *Meeting of the German Physical Society (DPG) 2006*, Dresden, Germany, March 27 – 31, **2006.**
100. **V. Harmandaris**, N.F.A. van der Vegt, K. Kremer "Hierarchical modeling of PS: from atomistic to coarse-grained simulations" *4th International Workshop on non-Equilibrium Thermodynamics and Complex Fluids*, Rhodes, Greece, September 3-7, **2006**.
101. **V. Harmandaris,** V.G. Mavrantzas, "Dynamics of thin polymer melt films near at a solid attractive surface through atomistic molecular dynamics simulations", (Poster) *International School of Solid State Physics34th Course: Computer Simulations in Condensed Matter: from Materials to Chemical Biology*, Erice, Italy, July 20 – August 1, **2005.**
102. **V. Harmandaris,** K. Daoulas, V.G. Mavrantzas, "Polyethylene dynamics in polyethylene/graphite interfaces", *European Polymer Conference 2005*, Moscow, Russia, June 26 – July 1, **2005.**
103. **V. Harmandaris,** K. Daoulas, V.G. Mavrantzas, "Atomistic simulation of the structure and dynamics of the polyethylene/graphite interface", *3rd International Conference for Computational Modeling and Simulation of Materials (CIMTEC)*, Acireale, Italy, May 30 – June 4, **2004.**
104. **V. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Atomistic molecular dynamics simulation of the self-diffusion of n-alkane melts and of binary n-alkane blends", *AIChE Annual Meeting*, San Francisco, November 16-21, **2003.**
105. **V. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Molecular dynamics simulation of the viscoelastic properties of long polymer melts: From Rouse to reptation theory", *AIChE Annual Meeting*, San Francisco, November 16-21, **2003.**
106. **V. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Molecular dynamics simulation of the viscoelastic properties of linear polymer melts", *Polymer Processing Society (PPS)*, Athens, September 14-17, **2003**.
107. **V. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Prediction of the viscoelastic properties of polymer from detailed molecular dynamics simulations and comparison against rheological measurements", *3rd Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean (EMCC-3)*, Thessaloniki, Greece, May 13-15, **2003.**
108. **V. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Prediction of the rheological properties of long polyethylene melts via atomistic molecular dynamics simulations", *3rd International Meeting of the Hellenic Society of Rheology*, Patras, Greece, June 10-14, **2001.**
109. **V. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Prediction of the viscoelastic properties of high-molecular weight polymer melts through molecular dynamics atomistic simulations", *3rd Panhellenic Chemical Engineers' Conference*, Athens, Greece, May 31-June 02, **2001**.
110. **V. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Prediction of the linear viscoelastic properties of long-chain polyethylene melts from detailed atomistic simulations on uniaxially stretched melt configurations", *XIII International Congress on Rheology*, Cambridge, UK, August 20-25, **2000**.
111. **V. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Atomistic modeling of viscoelasticity: simulation of stress relaxation upon cessation of steady-state elongational flow", *Summer School in Polymer Science and Technology*, Psathopirgos, Patras, Greece, September 5-9, **1999**.
112. **V. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Atomistic simulation of the stress relaxation experiment after cessation of steady-state uniaxial elongation", *2nd Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 27-29, **1999**.
113. **V. Harmandaris**, V.G. Mavrantzas, D.N. Theodorou, D.N. "From chemical structure to polymer

processing: Atomistic simulation of the viscoelasticity of linear polyethylene melts", *4th Panhellenic Conference on Polymers*, Patras, Greece, November 20-22, **1997**.

Representative presentations by others (speaker underlined)

114. P. Bačová**, V. Harmandaris**, " Computational Modeling of Star-shaped Polymer Materials ", 2nd BGU-FORTH/UoC Soft Matter workshop, Beer Sheva, Ben Gurion Univ., Israel, 25-27 February **2020**.
115. E. Kalligiannaki, G. Baxevani, A. Chazirakis and **V. Harmandaris**, "Systematic Coarse-Grained Models for Molecular Systems Using Entropy", *European Congress and Exhibition of Advanced Materials and Processes (EUROMAT 2019)*, Stockholm, Sweden, 1-5 September **2019**.
116. M. Arnittali, A. Rissanou, **V. Harmandaris**, "Structure Of Biomolecules through Molecular Dynamics Simulations", 8*th International Young Scientists Conference on Computational Science, YSC2019*, Heraklion, 24-28 June **2019**.
117. P. Bačová**, V. Harmandaris**, "Multi-scale Dynamic simulations of polymer nanocomposites with inorganic or polymer-based nanoparticles", *9th International Meeting of the Hellenic Rheology Society,* Samos, Greece, June 24-27, **2019**.
118. G. Baxevani, E. Kalligiannaki, **V. Harmandaris**, "Study of the transient dynamics of coarse-grained molecular systems with the path-space force-matching method", 8*th International Young Scientists Conference on Computational Science, YSC2019*, Heraklion, 24-28 June **2019**.
119. P. Bačová, E. Glynos, S. Anastasiadis, **V. Harmandaris**, "Computational design of nanostructured polymer materials", *European Polymer Congress 2019 (EPF 2019)*, Heraklion, Crete, Greece, 9-14 June, **2019**.
120. A. Behbahani, **V. Harmandaris**, "Structure and dynamics of stereoregular poly(methyl methacrylate) chains adsorbed on pristine and oxidized graphene via atomistic simulations", *European Polymer Congress 2019 (EPF 2019)*, Heraklion, Crete, Greece, 9-14 June, **2019**.
121. A. Rissanou, **V. Harmandaris**, "Properties of polymer melts and polymer/silica nanocomposites through multi-scale molecular simulations", *European Polymer Congress 2019 (EPF 2019)*, Heraklion, Crete, Greece, 9-14 June, **2019**.
122. M. Arnittali, A. Rissanou, **V. Harmandaris**, "Structure and self-assembly of biomolecules through Molecular Dynamics Simulations ", 12*th Panhellenic Chemical Engineers' Conference*, Salonica, Greece, 29-31 May, **2019**.
123. A. Rissanou, P. Bačová, **V. Harmandaris**, "Atomistic molecular dynamics simulations of multiphase polymer/graphene nanostructured systems", 12*th Panhellenic Chemical Engineers' Conference*, Salonica, Greece, 29-31 May, **2019**.
124. V. Raptis, **V. Harmandaris**, " Using coarse-grain and fully atomistic force fields to predict the properties of poly(lactate acid) via Molecular Dynamics simulations", 12*th Panhellenic Chemical Engineers' Conference*, Salonica, Greece, 29-31 May, **2019**.
125. P. Bačová, E. Glynos, **V. Harmandaris**, "Computational design of nanostructured polymer materials: atomistic simulations of self-segregated and self-assembled miktoarm star copolymers", *Annual European Rheology Conference*, Sorento, Ital, April 17-20, **2019**.
126. G. Kritikos, A. Chazirakis, P. Bačová, A. Rissanou, E. Kalligiannaki, and **V. Harmandaris**, "Hierarchical Multi-scale Computational Methodologies for the Study of Complex Molecular Systems", *The Twelfth International Conference on Advanced Engineering Computing and Applications in Sciences*, Athens, Greece, November 18-22, **2018**.
127. E. Kalligiannaki, M. Katsoulakis, P. Plechac, **V. Harmandaris**, "Path space force matching and relative entropy methods for coarse-graining molecular systems at transient regimes",*7th International Young Scientists Conference on Computational Science, YSC2018*, Heraklion, Crete, July 02-06, **2018**.
128. P. Bačová, A.N. Rissanou, **V. Harmandaris**, "Modelling of novel polymer materials through atomistic molecular dynamics simulations",*7th International Young Scientists Conference on Computational Science, YSC2018*, Heraklion, Crete, July 02-06, **2018**.
129. E. Kalligiannaki, **V. Harmandaris**, M. Katsoulakis, P. Plechac "From Atomistic to Systematic Coarse-graining of Molecular Systems", 2nd ECCOMAS, Thematic Conference on International Conference on Uncertainty Quantification in Computational Sciences and Engineering (UNCECOMP), Rhodes, Greece, June 15-17, **2017**.

130. A.J. Power, **V. Harmandaris**, "Atomistic Molecular Dynamics Simulations of Hybrid Polymer/Gold and Core-Shell Nanoparticle Systems", 11*th Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 25–27, **2017**.
131. (Poster) A.J. Power, **V. Harmandaris**, "Dynamics and Structure of Hybrid Polymer Nanocomposites with Core-Shell Nanoparticles", Eurofillers & Polymer Blends, Heraklion, Crete, Greece, April 23-27, **2017**.
132. (Poster) A. Tsourtis, E. Kalligiannaki, **V. Harmandaris**, "Parametrizing coarse grained models for molecular systems at equilibrium", Proceedings, *11th Hellenic Polymer Society International Conference,* Heraklion, Greece, November 03-05, **2016**.
133. (Poster) P. Bačová, A. Rissanou, **V. Harmandaris**, "Graphene based Polymer Nanostructured Materials through Molecular Simulations", Proceedings, *11th Hellenic Polymer Society International Conference,* Heraklion, Greece, November 03-05, **2016**.
134. (Poster) A. Rissanou, P. Bačová, **V. Harmandaris**, "Properties of Nanographene in Polymer Nanocomposites through All-atom Simulations", Proceedings, *11th Hellenic Polymer Society International Conference,* Heraklion, Greece, November 03-05, **2016**.
135. (Poster) V. Petrakis, A. Rissanou, **V. Harmandaris**, H. Papananou, K. Chrissopoulou, S. Anastasiadis, "Structural and Conformational Properties of Poly-(ethylene oxide)/Silica Nanocomposites through Simulations and Experiments", Proceedings, *11th Hellenic Polymer Society International Conference,* Heraklion, Greece, November 03-05, **2016**.
136. (Poster) A. Power, **V. Harmandaris** "Detailed Atomistic Molecular Dynamics Simulations of Hybrid Polymer /Core-Shell Nanoparticle Systems", Proceedings, *11th Hellenic Polymer Society International Conference,* Heraklion, Greece, November 03-05, **2016**.
137. A. Rissanou, P. Bačová, **V. Harmandaris**, "Atomistic Simulation of Graphene-Based Polymer Nanocompositess", *8th International Conference Times of Polymers and Conferences*, Ischia, Italy, June 19-23, **2016.**
138. E. Kalligiannaki, **V. Harmandaris**, M. Katsoulakis, P. Plechac "Coarse-graining Non-equilibrium systems and path space information theory", European Community on Computational Methods in Applied Sciences (ECCOMAS) Congress 2016, Crete, Greece, June 5-10, **2016**.
139. E. Kalligiannaki, M. Katsoulakis, P. Plechac, **V. Harmandaris**, " Optimizing Coarse-grained Models for Equilibrium and Non-equilibrium Molecular Systems: Force matching and Dynamical Force Matching", *International Workshop on Nonequilibrium Thermodynamics (IWNET)*, Hilvarenbeek, Netherlands, July 05–10, **2015.**
140. A. Tsourtis, I. Pantazis, M. Katsoulakis, **V. Harmandaris**, " Parametric Sensitivity Analysis for Stochastic Molecular Systems using Information Theoretic Metrics", 10*th Panhellenic Chemical Engineers' Conference*, Patras, Greece, June 04–06, **2015.**
141. A.J. Power, **V. Harmandaris**, "Structure and Dynamics of Hybrid Polymer/Nanocomposite Systems through Molecular Dynamics Simulations", 4th International Young Scientists Conference and Summer School, Athens, Greece, June 25 - July 3, **2015**.
142. (Poster) A.J. Power, **V. Harmandaris**, "Structure and Dynamics of Hybrid Polymer/Gold Nanoparticle Systems through Atomistic Molecular Dynamics Simulations”. Computational Trends in Solvation and Transport in Liquids", Julich, Germany, March 23-27, **2015**.
143. A. Rissanou, D. Tzeli, **V. Harmandaris**, "Self-assembly of Diphenylalanine and Chemically Modified Diphenylalanine Peptides on Various Solvents", 10*th Panhellenic Chemical Engineers' Conference*, Patras, Greece, June 04–06, **2015.**
144. A. Power, **V. Harmandaris**, "Structure and Dynamics of Hybrid Polymer/Gold Nanoparticle Systems through Atomistic Molecular Dynamics Simulations", 10*th Panhellenic Chemical Engineers' Conference*, Patras, Greece, June 04–06, **2015.**
145. A. Rissanou, **V. Harmandaris**, "Molecular Simulations of Polymer-Graphene Nanocomposites", *European Polymer Federation Congress 2015*, Dresden, Germany, June 21-26, **2015.**
146. P. Bačová, **V. Harmandaris**, "Dynamics of Functionalized Graphene Based Polymer Nanocomposites through Detailed Atomistic Simulations", *Annual European Rheology Conference,* Nantes, France, April 14-17, **2015**.
147. P. Bačová, A. Rissanou, **V. Harmandaris**, "Detailed Molecular Simulations of Functionalized Graphene Based Polymer Nanocomposites", *American Physical Society, APS March Meeting*, San Antonio, USA, March 02-06, **2015.**

148. A. Rissanou, **V. Harmandaris**, "Study of Polymer/Graphene Nanocomposites through Atomistic Molecular Dynamics Simulations", *American Physical Society, APS March Meeting*, San Antonio, USA, March 02-06, **2015.**
149. A. Power, **V. Harmandaris** "Properties of polymer/gold nanocomposites through atomistic molecular dynamics simulations", (Poster) *10th Hellenic Polymer Society Conference,* Patras, Greece, December 04-06, **2014**.
150. V.S. Petrakis, A.N. Rissanou, **V. Harmandaris**, K. Chrisopoulou, S. Anastasiadis "Atomistic molecular dynamics simulation study of a hybrid poly (ethylene oxide) / silica nanoparticle system", (Poster) *10th Hellenic Polymer Society Conference,* Patras, Greece, December 04-06, **2014**.
151. A. Rissanou, **V. Harmandaris**, "Molecular Simulations of graphene based polymer nanocomposite", *10th Hellenic Polymer Society Conference,* Patras, Greece, December 04-06, **2014**.
152. V.S. Petrakis, A.N. Rissanou, **V. Harmandaris**, K. Chrisopoulou, S. Anastasiadis "Atomistic Molecular Dynamics Simulation Study of Hybrid Poly(ethylene oxide) / Silica Nanoparticle Systems", (Poster) *30th Panhellenic Conference on Solid State Physics and Materials Science*, Heraklion, Greece, September 21-24, **2014**.
153. A. Power, I. Remediakis, **V. Harmandaris** "Properties of Polymer/Gold Nanocomposites Through Atomistic Molecular Dynamics Simulations", (Poster) *30th Panhellenic Conference on Solid State Physics and Materials Science*, Heraklion, Greece, September 21-24, **2014**.
154. K. Johnston, K. Kremer, **V. Harmandaris**, "Confined polystyrene films between gold surfaces", *American Physical Society, APS March Meeting*, Boston, Massachusetts, USA, February 27-March 2, **2012.**
155. Won Bo Lee, **V. Harmandaris**, D. Fritz, K. Kremer, "Dynamics of polystyrene (PS) melts: multi-scale molecular dynamic approach", Proceedings, *American Physical Society, APS March Meeting*, Pittsburgh, Pennsylvania, USA, March 16-20, **2009.**
156. D. Fritz, **V. Harmandaris**, D. Reith, N.F.A. van der Vegt, K. Kremer "Structure and dynamics of coarse grained polystyrene melts", (Poster) *German Physical Society (DPG)*, Berlin, Germany, February 25-29, **2008.**

Funding-Grants (during the last 10 years)

1. **H2020-MSCA-IF-2020, HORIZON 2020, EU research and innovation programme**, 2021–2023. Title: "*Mechanical Properties of Polymer Nanocomposites via Multi-scale Modeling: Towards Non-classical Properties (NANOMEC)*". MSCA Fellow: Dr. Hilal Reda, Role: PI of the Host institution. Budget of the grant: 157.941 Euro.
2. **H2020-MSCA-COFUND-2020, HORIZON 2020, EU research and innovation programme**, 2021–2025. Title: "*Enabling the Next-Generation of Computational Physicists and Engineers (ENGAGE)*". Role: Team Leader. Grant request: 1.681.440, Total budget of the project: 3.362.880 Euro.
3. **Era Chair, HORIZON 2020, EU research and innovation programme**, 2019–2024. Title: "*Modeling and Simulation for Engineering Applications (SimEA)*". Role: PI. Budget of the grant: 2.500.000 Euro.
4. **ΕΛΙΔΕΚ**, Greece, 2020–2023. Title: "*Polymer Dynamics Under 2-d Confinement*". Role: Team Member (PI: G. Floudas). Budget of the grant: 200.000 Euro.
5. **Industry Funding**, Goodyear, Akron, USA, 2017–2022. Title: "*Computational Design of Tire Materials*". Role: PI. Budget of the grant: 1.300.000 USA Dollars.
6. **«Ερευνώ – Δημιουργώ – Καινοτομώ»,** GSRT, Greece, 2018–2021. Title: "*Bio-waste to Bio-plastic (B2B)*". Role: Team Leader. Budget of the team: 120.000 Euro (Overall budget of the grant: 1.000.000 Euro).
7. **KRHPIS II**, GSRT, Greece, 2017–2021. Title: "*Advanced Research Activities in Biomedical Technology and Agricultural (BITAΔ)*". Role: Team Leader. Budget of the team: 25.000 Euro (Overall budget of the grant: 1.467.000 Euro).
8. **KRHPIS II**, GSRT, Greece, 2017–2021. Title: "*Materials and Processes for Applications in Energy and Environment (AENAO)*". Role: PI of the IACM/FORTH. Budget of the team: 25.000 Euro (Overall budget of the grant: 1.084.900 Euro).

9. **ELKE, UOC**, 2016–2018, Title**: "***Multiscale Computational Modeling of Hybrid Polymer / Nanoparticle Systems***".** Principal Investigator (PI): V. Harmandaris. Budget of the grant: 15.000 Euro.
10. **ARISTEIA II**, GSRT, Greece, 2014–2015. Title: "*Hierarchical Multi-scale Modeling of Complex Materials*". Role: Principal Investigator (PI). Budget of the grant: 200.000 Euro.
11. **KRHPIS I**, GSRT, Greece, 2013–2015. Title: "*Advanced – Smart Materials*". Role: Team Leader. 30.000 Euro (Overall budget of the grant: 1.573.000 Euro).
12. **THALIS**, GSRT, Greece, 2012–2015. Title: "*Analysis, modeling and simulations of complex systems*". Role: Team Leader, PI during 02-09/15. Budget of the grant: 600.000 Euro.
13. **THALIS**, GSRT, Greece, 2012–2015. Title: "*Self-assembly and dynamics in metastable states. From molecular and supramolecular to mesoscopic systems*". Role: Team Member (PI: G. Floudas). Budget of the grant: 600.000 Euro.
14. **DFG SPP1369**, 2008–2011. Title: "*Dynamics of polymer melts near solid interfaces*", Role: Principal Investigator (PI), together with H. Duran. Budget of the grant: 200.000 Euro. Duration (starting/ending) dates: 07/2008 – 06/2014.
15. **ELKE, UOC**, 2011–2013, Title: "*Hierarchical multi-scale modeling of polymer nanocomposites*". Principal Investigator (PI): V. Harmandaris. Budget of the grant: 15.000 Euro.
16. **NSF, USA**, 2008–2013. Title: "*From nanoscale simulation to process engineering: Building a network for understanding polymer dynamics*". Role: International collaborator (PI: B. Edwards). Budget of the grant: 100.000 Euro.

Citations (ISI, Web of Science)
(Till 30/06/2021):

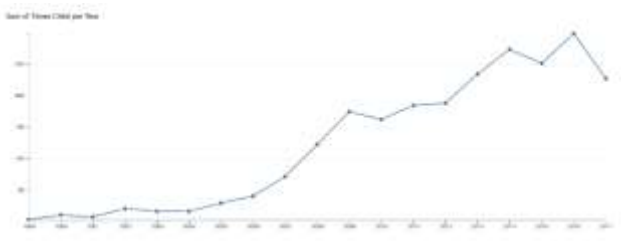
Total: **3515**

Clean (non-self): **3082**

Average Citations per article: **38.6**

h-Index: 31
(Beam plot: Overall median **81st percentile**)

Citations in Each Year



Citations (Google Scholar) (Till 31/05/2020):

Total:	**4600**	(since 2016: **2124**)
h-index:	**34**	(since 2016: **24**)
i10-index:	**59**	(since 2016: **51**)

ResearcherID: B-2958-2009, ORCID: 0000-0002-9613-7639.

Teaching

Courses taught
a) Graduate

1. "Modeling and Simulation for Scientific Applications", CaSToRC, CyI, Spring **2020-2021**.
2. "Frontiers & Methodologies in Computational Sciences" (joined course), CaSToRC, CyI, Spring **2020-2021**.
3. "Statistical Inference and Machine Learning for Molecular Systems", (with E. Kalligiannaki) Department of Mathematics and Applied Mathematics, University of Crete, Spring **2019-2020**.

4. "Mathematical Modeling in Natural Sciences", Department of Mathematics and Applied Mathematics, University of Crete, Spring **2018-2019**.
5. "Monte Carlo Methods", Department of Mathematics and Applied Mathematics, University of Crete, Spring **2015-2016**.
6. "Statistical Mechanics", Department of Mathematics and Applied Mathematics, University of Crete, Spring **2014-2015.**
7. "Scientific Computing", Department of Applied Mathematics, University of Crete, Spring **2013-2014.**

b) Undergraduate

8. "Mathematics II", Department of Chemistry, University of Crete, Spring **2019-2020**; **2018-2019;** Spring **2014-2015.**
9. "Applied Statistics", Department of Mathematics and Applied Mathematics, University of Crete, Fall **2019-2020**; Department of Applied Mathematics, University of Crete, Spring **2009-2010.**
10. "Optimization", Department of Mathematics and Applied Mathematics, University of Crete, Spring **2018-2019**.
11. "General Mathematics I", Department of Materials, University of Crete, Fall **2019-2020**; Fall **2018-2019**.
12. "Calculus I", Department of Mathematics and Applied Mathematics, University of Crete, Fall **2017-2018**.
13. "Introduction to Programming: Python II", Department of Mathematics and Applied Mathematics, University of Crete, Spring **2015-2016**; Spring **2016-2017.**
14. "Mathematical Modeling", Department of Mathematics and Applied Mathematics, University of Crete, Fall **2016-2017**.
15. "Mathematical Biology", Department of Mathematics and Applied Mathematics, University of Crete, Fall **2015-2016, 2011-2012**.
16. "Mathematical Modeling and Numerical Simulations", Department of Mathematics and Applied Mathematics, University of Crete, Fall **2014-2015.**
17. "Physics I", Department of Mathematics and Applied Mathematics, and Department of Computer Science, University of Crete, Fall **2014-2015.**
18. "Introduction in Monte Carlo Methods", (Undergraduate and Graduate Course) Department of Applied Mathematics, University of Crete, Spring **2013-2014**, Spring **2012-2013**, Spring **2011-2012.**
19. "Linear and Non-linear Programming", Department of Mathematics and Applied Mathematics, University of Crete, Fall **2013-2014.**
20. "Introduction to *C*", Department of Applied Mathematics, University of Crete, Fall **2012-2013**.
21. "Data Structures", Department of Applied Mathematics, University of Crete, Spring **2010-2011**.
22. "Parallel Programming", Department of Applied Mathematics, University of Crete, Fall **2009-2010,** Fall **2010-2011**.

Teach Assistant as PhD student (Department of Chemical Engineering, University of Patras, Greece): "Introduction to Fortran", Fall **1997, 1998, 1999;** "Numerical Analysis", Spring **1999**; "Polymers Laboratory", Spring **1998.**

Managerial Experience

Member of the Research Committee of the University of Crete (ΕΛΚΕ): 06/2016 – 09/2020

Administrative and Departmental Committee Duties at Dept. of Mathematics and Applied Mathematics, University of Crete

Member of the Departmental Committee on Computing and Software: 01/2015 – 09/2021
Member of the Departmental Committee on the Building: 01/2016 – 09/2021
Member of the Departmental Committee on Graduate Programme: 01/2013 – 09/2018
Scientific Responsible of the Department for Internship – "Praktiki Askhsh": 01/2016 – 09/2018
Member of the Departmental Committee on Internship – "Praktiki Askhsh": 01/2012 – 12/2015
Member of the Departmental Committee on Evolvement, Planning and Organization: 03/2011 – 03/2013

Graduate Students Advised and Postdoctoral Scholars

Current Postdoctoral Scholars:
1. Dr. H. Reda (04/2021 – till now)
2. Dr. P. Katsamba (08/2020 – till now)
3. Dr. Petra Bačová (10/2014 – 11/2015; 05/2017 – till now))
4. Dr. Anastasia Rissanou (01/2015 – till now)
5. Dr. Alireza F. Behbahani (03/2019 – till now)

PhD Students:
1. Lefteris Christofi (09/2020 – till now)
2. Nikolas Patsalidis (09/2020 – till now)
3. Eiriin Gkolfi (03/2020 – till now)
4. Antonis Chazirakis (07/2019 – till now)
5. Maria Arnittali (06/2019 – till now)
6. Georgia Baxevani (06/2019 – till now)
7. Albert Power (09/2015 – till now)

Master Students:
1. Vasia Kyrierh
2. Vasiliki Rizou

Current Diploma Students:

Previous Postdoctoral Scholars:
1. Dr. A. Mahmood (10/2020 – 09/2021)
2. Dr. Vasilis Raptis (03/2019 – 12/2020)
3. Dr. Evangelia Kalligiannaki (10/2013 – 10/2015)
4. Dr. Karen Johnston (01/2010 – 06/2013)

Degrees Awarded:
PhD:
1. Anastasios Tsourtis, Department of Mathematics and Applied Mathematics, University of Crete, Thesis title: "*Mathematical and computational modeling of complex molecular systems in multiple scales*", graduated in 02/2017.
2. Alireza Foorazani (Department of Chemical Engineering, University of Tehran, Iran, Co-advisor, Advisor: M. Baez, Thesis title: "*Atomistic Simulations of Polymer/Graphene Interfacial Systems*", graduated in 02/2019).

Master:
1. Dimosthenis Vallis, (with S. Komineas) Department of Mathematics and Applied Mathematics, University of Crete, graduated in 09/2021.
2. Eleytheria Stavropoulou, Department of Mathematics and Applied Mathematics, University of Crete, graduated in 09/2020.

3. Eirini Gkolfi, Department of Mathematics and Applied Mathematics, University of Crete, graduated in 10/2019.
4. Maria Arnittali, Department of Mathematics and Applied Mathematics, University of Crete, graduated in 11/2018.
5. Georgia Baxevani, Department of Mathematics and Applied Mathematics, University of Crete, graduated in 11/2018.
6. Sofianna Kavousanou, Department of Mathematics and Applied Mathematics, University of Crete, graduated in 11/2017.
7. Antonis Chazirakis, Department of Mathematics and Applied Mathematics, University of Crete, graduated in 10/2017.
8. Virginia Apostolopoulou, Department of Mathematics and Applied Mathematics, University of Crete, graduated in 02/2017.
9. Areth Zervou, Department of Mathematics and Applied Mathematics, University of Crete, graduated in 07/2016.
10. Maria Panoukidou, Department of Mathematics and Applied Mathematics, University of Crete, graduated in 09/2015.
11. Vyrwnas Petrakis, Department of Chemistry, University of Crete, graduated in 09/2015.
12. Despoina Tzeli, Department of Materials, University of Crete, graduated in 09/2015.
13. Albert Power, Department of Materials, University of Crete, graduated in 08/2015.

Diplomas:

(Department of Mathematics and Applied Mathematics, University of Crete)

2019-20: Agapi Zhsh, Anastasia Papadaki;
2018-19: Eirini Kostoglou;
2017-18: Panagiwta Siachouli, Eleytheria Stavropoulou;
2016-17: Katerina Arkavlh, Panagiwta Keramea;
2015-16: Germanos Chatziathanasiou, Alexander Kovalenko, Katerina Avramidou;
2014-15: Virginia Apostolopoulou, Maria Panoukidou, Alexia Katsara;

(Department of Applied Mathematics, University of Crete)

2013-14: Antonis Chazirakis, Myron Gourlis, Maria Demetzou, Kostas Koskoletos,
2012-13: Despoina Tzeli, Albert Power;
2011-12: Eirinh Kakari

Member of PhD/Master/Diploma Committee

PhD Students:

1. Dimitris Stefanakis (Department of Materials, University of Crete, Advisor: I. Remediakis, member of primary three-member PhD Committee, 2017 – Today).
2. Dimitris Mintis (Department of Chemical Engineering, University of Patras, Advisor: V. Mavrantzas, graduated in 07/2020).
3. Michael Goutsoulas (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: N. Efremidis, graduated in 04/2020).
4. Eleytherios Koufakis (Department of Materials, University of Crete, Advisor: M. Vamvakaki, graduated in 12/2019).
5. Lucille Chambon (Department of Materials, University of Crete, Advisor: D. Vlassopoulos, graduated in 07/2019).
6. Daphne Davelou (Department of Materials, University of Crete, Advisor: I. Remediakis, graduated in 07/2019).
7. Flora Tsourtou (Department of Chemical Engineering, University of Patras, Advisor: V. Mavrantzas, graduated in 06/2019).
8. Costas Smaragdakis (Department of Mathematics and Applied Mathematics, University of Crete, graduated in 04/2019).
9. Panagiotis Tzounis (Department of Chemical Engineering, National Technical University of Patras, Advisor: D. Theodorou, graduated in 03/2019).

10. Orestis Ziogos (Department of Chemical Engineering, National Technical University of Patras, Advisor: D. Theodorou, graduated in 03/2018).
11. Salvatore Costanzo (Department of Materials, University of Crete, Advisor: D. Vlassopoulos, graduated in 02/2017).
12. Emmanouil Daskalakhs (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: C. Tsogka, graduated in 07/2016).
13. Michael Apostoloupoulos (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: C. Tsogka, graduated in 06/2016).
14. Aristea Maniadaki (Department of Materials, University of Crete, Advisor: G. Kopidakis, graduated in 10/2015).
15. Elnaz Hajizadeh Darzehkonan (Thesis Examiner, Department of Materials, University of Crete, Advisor: G. Floudas, graduated in 12/2014).
16. Eleni Androulaki (Department of Materials, University of Crete, Advisor: I. Economou, graduated in 03/2014).
17. Giwrgos Arabatzis (Department of Applied Mathematics, University of Crete, Advisor: M. Katsoulakis, graduated in 01/2014).
18. Alexandros Anastasiou (Department of Chemical Engineering, University of Patras, Advisor: B. Mavrantzas, graduated in 12/2013).

External PhD Evaluator:

19. Parya Keyvani (Chemical and Biological Engineering, The University of British Columbia (Vancouver), Canada. Advisor: S. Chatzikiriakos, Thesis title: "*Ionic Diodes Based on Cellulose Nanocrystals (CNC) and Related Rheological Studies*", graduated in 09/2021).
20. Elnaz Hajizadeh Darzehkonani (Department of Mathematics, Faculty of Science, Engineering and Technology, and Centre for Molecular Simulation, Swinburne University of Technology, Victoria, Australia. Advisor: B. Todd, graduated in 03/2015).

Master Students:

1. *Georgios Papadomichelakis* (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: T. Katsaounis, graduated in 1/10/2021).
2. *Maria Daskalaki* (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: M. Pavlidis, to be graduated in 21/09/2021).
3. *Dimitris Hatzogiannakis* (Department of Chemistry, University of Crete, Advisor: S. Anastasiadis, graduated in 16/10/2020).
4. *Anna Frixou* (CaSToRC, The Cyprus Institute (CyI), Cyprus, Advisor: C. Papanicolas, graduated in 07/10/2020).
5. *Angeliki Boubaki* (Department of Materials, University of Crete, Advisor: I. Remediakis, graduated in 17/07/2020).
6. *Eleytherios Christofi* (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: T. Katsaounis, graduated in 14/07/2020).
7. *Petros Ntivanak* (Department of Materials, University of Crete, Advisor: A. Mitraki, graduated in 04/02/2020).
8. *Niki Iliadi* (Department of Materials, University of Crete, Advisor: M. Vamvakaki, graduated in 10/2018).
9. *David Bachman* (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: S. Komineas, graduated in 17/07/2018).
10. *Konstantinos Pappas* (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: I. Platis, graduated in 24/04/2016).
11. *Venetia Kokarakh* (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: G. Karalh, graduated in 31/03/2016).
12. *Athanasios Koulouris* (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: S. Komineas, graduated in 12/2015).
13. *Mixalhs Gourzoulidhs* (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: M. Plexousakis, graduated in 11/2015).

14. *Xristina Lazaridou* (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: A. Tzavaras, graduated in 06/2015).
15. *Alexandra Roussou* (Department of Physics, University of Crete, Advisor: S. Komineas, graduated in 12/2014).
16. *Giwta Kotsopoulou* (Department of Materials, University of Crete, Advisor: I. Remediakis, graduated in 03/2014).

Diploma Students:
2018-19: Maria Kotrotsiou Korosidhs (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: G. Zourais, graduated in 10/2019);
2017-18: Charalambos Korosidhs (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: M. Plexousakis, graduated in 07/2018);
2016-17: Magdalhnh Drougka (Department of Computer Science, University of Crete, Advisor: A. Mouxtarhs, graduated in 04/2017); V. Vouvoutsis (Department of Biology, University of Crete, Advisor: K. Sidiropoulou, graduated in 07/2017); Afrodith Dhmhtriadh (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: I. Platis, graduated in 07/2017); Elena Tsagkaris (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: I. Platis, graduated in 05/2017);
2015-16: Dimitra Petsa (Department of Biology, University of Crete, Advisor: K. Lyka, graduated in 03/2016; Maria Proestakh (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: P. Rosakis, graduated in 07/2016; Andrianna Manousidakh (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: M. Plexousakhs, graduated in 07/2016); Konstantinos Sgontzos (Department of Computer Science, University of Crete, Advisor: Y. Tzitzikas, graduated in 06/2016); 2) Michalis Sgouromallhs (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: I. Platis, graduated in 06/2016); Eleftherios Dimitrakhs (Department of Computer Science, University of Crete, Advisor: Y. Tzitzikas, graduated in 06/2016);
2014-15: Vasiliki Filippa (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: I. Platis, graduated in 10/2015); Stavros Kollias (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: T. Katsaounis, graduated in 07/2015); Dhmhtra Pagkalou (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: E. Tzanakh, graduated in 06/2015); Panagiwta Zwtou (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: M. Taroudakis, graduated in 03/2015); Kallioph Domalakh (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: M. Taroudakis, graduated in 03/2015);
2013-14: Stavros Giannoukakos (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: A. Tzavaras, graduated in 10/2014; Georgia Sfakianakh (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: M. Plexousakhs, graduated in 06/2014); Mirto Galanopoulou (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: D. Tsagkarogiannis, graduated in 09/2013); Danai Eleytheriou (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: D. Antonopoulou, graduated in 07/2013);
2009-2012: Panagiotis Stamatopoulos (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: C. Tsogka, graduated in 11/2012); Konstantinos Lazaridis (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: P. Rosakis, graduated in 10/2012; Athina Vasilakh (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: G. Karalh, graduated in 09/2012); Eirini Leivadarou (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: G. Karalh, graduated in 09/2012); Savvas Kaloudis (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: G. Karalh, graduated in 06/2012); Nikolaos Papanikolaou (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: G. Karalh, graduated in 02/2012); Nikolaos Kountouris (Department of Mathematics and Applied Mathematics, University of Crete, Advisor: G. Karalh, graduated in 05/2011); Amalia Leivadiwtou (Department of Biology, University of Crete, Advisor: K. Lyka, graduated in 02/2011.