VAGELIS A. HARMANDARIS

Office Address
Department of Applied Mathematics
University of Crete
Heraklion, GR-71409
Greece
&
Max Planck Institute for Polymer Research
Theory Group, Mainz, D-55021, Germany
Tel.: +30-2810-393735
Fax: +30-2810-393701
e-mail: vagelis@tem.uoc.gr
web page: http://www.tem.uoc.gr/~vagelis

Home Address
Panepistimiou 49
Heraklion, GR-71500
Greece

Research Interests

Multiscale Modeling: atomistic simulations, hierarchical molecular modeling, mesoscopic modeling, molecular dynamics, Monte Carlo, Brownian dynamics, field theory simulations, mathematical coarse-graining, model reduction, ab-initio DFT calculations..

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

Thermodynamics: Statistical mechanics, statistical thermodynamics, non-equilibrium thermodynamics.

Polymers: rheology and microscopic modelling, fluid-flow deformation dynamics, polymer/solid interfaces, grafted polymers, branched polymers, graphene based polymer nanocomposites.

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

Professional Experience

Assistant Professor (September 2009 - Today)
Department of Applied Mathematics, University of Crete, Greece

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

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)

Honors and Awards

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

Referee

American Chemical Society (Macromolecules, Langmuir), American Physical Society (Physical Review Letters, Physical Review E), Royal Society of Chemistry (Soft Matter, Physical Chemistry Chemical Physics, 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), Applied Surface Science, Journal of Nanoscience and Nanotechnology.

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).

Leisure Activities

Literature and poetry reading, music, playing basketball

Personal

Date of birth: November 3, 1973
Marital status: Married
Citizenship: Hellenic

Publications in Refereed Journals

1. K. Johnson, **V.A. 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.

2. K. Johnson, **V.A. 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.

3. D. Fritz, K. Koschke, **V.A. 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.

4. **V.A. Harmandaris**, G. Floudas, K. Kremer, "Temperature and pressure dependence of polystyrene dynamics through molecular dynamics simulations and experiments", *Macromolecules* **2011**, *44*, 393-402.

5. C. Baig, **V.A. Harmandaris** "Quantitative Analysis on the Validity of a Coarse-Grained Model for Nonequilibrium Polymeric Liquids under Flow", *Macromolecules*, **2010**, *43*, 3156-3160.

6. D. Fritz, **V.A. 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.

7. **V.A. Harmandaris**, K. Kremer, "Predicting polymer dynamics at multiple length and time scales", *Soft Matter*, **2009**, *5*, 3920-3926.

8. T. Cherdhirankorn, **V.A. 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.

9. **V.A. Harmandaris**, K. Kremer, "Dynamics of polystyrene melts through hierarchical multiscale simulations", *Macromolecules* **2009**, *42*, 791-802.

10. T. Mulder, **V.A. Harmandaris**, A.V. Lyulin, N.F.A. van der Vegt, K. Kremer, M.A.J. Michels, "Structural properties of atactic polystyrene of different thermal history obtained from a multi-scale simulation", *Macromolecules* **2009**, *42*, 384-391.

11. T. Mulder, **V.A. Harmandaris**, A.V. Lyulin, N.F.A. van der Vegt, M.A.J. Michels, "Molecular simulation via connectivity-altering Monte Carlo and Scale-jumping methods: Application to amorphous polystyrene", *Macrom. Theory Simul.* **2008**, *17*, 393-402.

12. T. Mulder, **V.A. Harmandaris**, A.V. Lyulin, N.F.A. van der Vegt, B. Vorselaars, M.A.J. Michels, "Equilibration and deformation of amorphous polystyrene: Scale-jumping simulation approach", *Macrom. Theory Simul.* **2008**, *17*, 290-300.

13. G. Tsolou, **V.A. Harmandaris**, V.G. Mavrantzas, "Molecular dynamics simulation of temperature and pressure effects on the intermediate length scale dynamics and zero shear rate viscosity of cis-1,4-polybutadiene: Rouse mode analysis and dynamic structure factor spectra", *J. Non-Newt. Fl. Mech.* **2008**, *152*, 184.

14. **V.A. Harmandaris**, D. Reith, N.F.A. van der Vegt, K. Kremer, "Comparison between coarse-graining models for polymer systems: Two mapping schemes for polystyrene", *Macrom. Chem. and Phys*. **2007**, *208*, 2109.

15. **V.A. Harmandaris**, N. Adhikari, N.F.A. van der Vegt, K. Kremer, R.Voelkel, C.C. Liew, H. Weiss, "Ethylbenzene diffusion in polystyrene: United atom atomistic/coarse grained simulations and experiments", *Macromolecules*, **2007**, *40*, 7026.

16. B. Reynolds, G. Illya, **V.A. Harmandaris**, M.M. Müller, K. Kremer, M. Deserno, "Mediated interactions between colloids adsorbed on a biological membrane", *Nature* **2007**, *447*, 461. Also in News and Views, Nature **2007**,*447*, 387. Also featured in the Virtual Journal of Biological Physics Research, June 1, 2007 issue.

17. O. Alexiadis, **V.A. Harmandaris**, V. Mavrantzas, L. de la Sitte, "Atomistic simulation of alkanethiol self-assembled monolayers on different metal surfaces via a quantum first-principles parameterization of the sulfur-metal interaction", *J. Phys. Chem. C* **2007**, *111*, 6380.

18. **V.A. Harmandaris**, M. Deserno, "A novel method for measuring the bending rigidity of model lipid membranes by simulating tethers", *J. Chem. Phys*. **2006**, *125*, 204905. Also featured in the Virtual Journal of Biological Physics Research, December 1, 2006 issue.

19. **V.A. Harmandaris**, N. Adhikari, N.F.A. van der Vegt, K. Kremer "Hierarchical modeling of polystyrene: From atomistic to coarse-grained simulations", *Macromolecules* **2006**, *39*, 6708.

20. G. Tsolou, **V.A. Harmandaris**, V.G. Mavrantzas, "Temperature and pressure effects on local structure and

chain packing in cis-1,4-polybutadiene from detailed molecular dynamics simulations", *Macrom. Theory Simul.* **2006**, *15*, 381.

21. G. Tsolou, **V.A. Harmandaris**, V.G. Mavrantzas, "Atomistic molecular dynamics simulation of the temperature and pressure dependences of local and terminal relaxations in cis-1,4-polybutadiene", *J. Chem. Phys*., **2006**, *124*, 084906.

22. C. Baig, B.J. Edwards, D.J. Keffer, H.D. Cochran, **V.A. Harmandaris** "Rheological and structural studies of linear polyethylene melts under planar elongational flow using nonequilibrium molecular dynamics simulations", *J. Chem. Phys*., **2006**, *124*, 084902.

23. K. Daoulas, D.N. Theodorou, **V.A. Harmandaris**, N.G. Karayiannis, V.G. Mavrantzas, "Self-consistent field study of compressible semiflexible melts adsorbed on a solid substrate and comparison with atomistic simulations", *Macromolecules*, **2005**, *38*, 7134-7149.

24. **V.A. Harmandaris**, K. Daoulas, V.G. Mavrantzas, "Molecular dynamics simulation of a polymer melt/solid interface: Local dynamics and chain mobility in a thin film of polyethylene melt adsorbed on graphite", *Macromolecules*, **2005**, *38*, 5796-5809.

25. K. Daoulas, **V.A. Harmandaris**, V.G. Mavrantzas, "Detailed atomistic simulation of a polymer melt / solid interface: Structure, density and conformation of a thin polyethylene melt film adsorbed on graphite", *Macromolecules*, **2005**, *38*, 5780-5795.

26. **V.A. Harmandaris**, V.G. Mavrantzas, D.N. Theodorou, M. Kröger, J. Ramírez, H.C. Öttinger, D. Vlassopoulos, "Dynamic crossover from Rouse to entangled polymer melt regime: Signals from long, detailed atomistic molecular dynamics simulations, supported by rheological experiments", *Macromolecules*, **2003**, *36*, 1376-1387.

27. **V.A. Harmandaris**, D. Angelopoulou, V.G. Mavrantzas, D.N. Theodorou, "Atomistic molecular dynamics simulation of diffusion in binary n-alkane/polyethylene melts", *J. Chem. Phys*., **2002**, *116*, 7656-7665.

28. **V.A. Harmandaris**, M. Doxastakis, V.G. Mavrantzas, D.N. Theodorou, "Detailed molecular dynamics simulation of the self-diffusion of n-alkane and cis-1,4 polyisoprene oligomer melts", *J. Chem. Phys*., **2002**, *116*, 436-446.

29. **V.A. Harmandaris**, V.G. Mavrantzas, D.N. Theodorou, "Atomistic molecular dynamics simulations of stress relaxation upon cessation of steady-state uniaxial elongational flow", *Macromolecules*, **2000**, *33*, 8062-8076.

30. **V.A. Harmandaris**, V.G. Mavrantzas, D.N. Theodorou, "Atomistic molecular dynamics simulations of polydisperse linear polyethylene melts", *Macromolecules*, **1998**, *31*, 7934-7943.

Publications Submitted or in Preparation

31. **V.A. Harmandaris**, G. Floudas, K. Kremer, "Dynamic Heterogeneity in Fully Miscible Blends of Polystyrene with Oligostyrene", submitted.

32. T. Rissanou, **V.A. Harmandaris**, "Structure and Dynamics of Poly(methyl-methacrylate)/Graphene systems through Atomistic Molecular Dynamics Simulations", submitted.

33. **V.A. Harmandaris**, M. Doxastakis, "Molecular Dynamics of Polyisoprene/Polystyrene Oligomer Blends: The role of self-concentration and fluctuations on blend dynamics", submitted.

34. T. Rissanou, E. Georgilis, M. Kasotaskis, A. Mitraki, **V.A. Harmandaris**, "Effect of Solvent on the Self-Assembly of Dialanine and Diphenylalanine Peptides", submitted.

35. M. Gianneli, K. Koynov, S. Brueckner, **V. Harmandaris**, E. Petrakis, I. M. Aslanides, J. Vetter, U. Jonas, "Direct Measurement of Riboflavin-5-phosphate Spatio-temporal Distribution in the Corneal Stroma", to be submitted.

Books and Chapter in Books

1. **V.A. Harmandaris,** M. Katsoulakis, "Computational and mathematical hierarchical modeling of molecular systems", in preparation, **2012.**

2. **V.A. Harmandaris,** V.G. Mavrantzas, "Atomistic Molecular Dynamics Simulation of Segmental Dynamics in Molten Polyethylene and Comparison with Experimental Data", Chapter in Book "Recent Research Topics and Developments in Chemical Physics: From Nanoscale to Macroscale", Edited by A.F. Terzis and E. Paspalakis, Research Signpost, India, **2009.**

3. **V.A. Harmandaris,** V.G. Mavrantzas, "Molecular Dynamics Simulations of Polymers", Chapter in Book "Simulation Methods for Polymers", Edited by M.J. Kotelyanskii and D.N. Theodorou, Marcel Dekker, New York, **2004.**

4. **V.A. Harmandaris,** "Atomistic Molecular Dynamics Simulations of Polymer Melt Viscoelasticity", Ph.D. Thesis, University of Patras, Patras, **2002**.

Publications in Conference Proceedings

1. A. Rissanou, **V.A. Harmandaris**, "Properties of polystyrene/graphene systems through detailed atomistic simulations", Proceedings, *GrapHEL, A European Conference/Workshop on the Synthesis, Characterization and Applications of Graphene*, Mykonos Greece, September 27-30, **2012**.
2. **V.A. Harmandaris**, C. Baig "Hierarchical modeling of polymers under non-equilibrium conditions: from atomistic to coarse-grained models", Proceedings, *XVIth International Congress on Rheology*, Lisbon, Portugal, August 5-10, **2012**.
3. **V.A. 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**.
4. K. Johnston, K. Kremer, **V.A. Harmandaris**, "Confined polystyrene films between gold surfaces", *American Physical Society, APS March Meeting*, Boston, Massachusetts, USA, February 27-March 2, **2012.**
5. **V.A. Harmandaris**, "Multi-scale simulations of fluid/solid hybrid composite systems", Proceedings, *18th International Conference on composite materials*, Busan, Jeju Island, Korea, August, 20-26, **2011**.
6. **V.A. Harmandaris**, "Structure and dynamics of non-equilibrium polymer melts through hierarchical multi-scale dynamic simulations", Proceedings, *6th Hellenic Society Rheology 2011*, Athens, Greece, July 27-30, **2011**.
7. **V.A. Harmandaris**, "A novel method for measuring the bending and the Gaussian rigidity of multi-component membranes by simulating tethers", Proceedings, *International Soft Matter Conference 2010, ISMC*, Granada, Spain, July 04-08, **2010**.
8. **V.A. Harmandaris**, "Multiscale modeling of polymers under equilibrium and non-equilibrium conditions: from atomistic to coarse-grained models", Proceedings, *International Soft Matter Conference 2010, ISMC*, Granada, Spain, July 04-08, **2010**.
9. **V.A. Harmandaris** and K. Kremer, "Polymer/Solid Interfaces Through Multi-scale Simulations", Proceedings, *17th Conference on Composite Materials, ICCM*, Edinburgh, Scotland, July 27-31, **2009**.
10. Won Bo Lee, **V.A. 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.**
11. **V.A. Harmandaris** and K. Kremer, "Dynamics of entangled polystyrene through hierarchical multi-scale simulations", Proceedings, *7th Hellenic Polymer Conference*, Ioannina, Greece, September 28-October 01, **2008**.
12. **V.A. Harmandaris** and K. Kremer, "Structure and Dynamics of Polymers Through Hierarchical Dynamic Simulations", Proceedings, *XXIV Panhellenic Conference on Solid State Physics and Materials Science*, Heraklion, Greece, September 21-24, **2008**.
13. N. van der Vegt, **V.A. Harmandaris**, B. Hess, K. Kremer, T.A. Ozal, C. Peter, "Multiscale simulations of polymer permeation", Proceedings, *AIChE Summer Meeting*, New Orleans, April 6-10, **2008**.
14. D. Fritz, **V.A. Harmandaris**, D. Reith, N.F.A. van der Vegt, K. Kremer "Structure and dynamics of coarse grained polystyrene melts", Proceedings, *German Physical Society (DPG)*, Berlin, Germany, February 25-29, **2008**.
15. B. Reynolds, G. Illya, **V.A. Harmandaris**, M.M. Müller, K. Kremer, M. Deserno, "Mediated interactions between colloids adsorbed on a biological membrane", Proceedings, *Biophysical Society Annual Meeting*, Long Beach, California, February 2-6, **2008**.
16. **V.A 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", Proceedings, *AIChE Annual Meeting*, San Francisco, November 16-21, **2003.**

17. D. Reith, **V.A. Harmandaris**, N.F.A. van der Vegt, K. Kremer "Hierarchical modeling of PS: from atomistic to coarse-grained simulations", Proceedings, *AIChE Annual Meeting*, Salt Lake City, November 4-9, **2007**.
18. D. Reith, **V.A. Harmandaris**, N.F.A. van der Vegt, K. Kremer "Structural and dynamical properties of Polystyrene determined by coarse-graining MD simulations", Proceedings, SOCOBIM, Terrasini, Italy, July 15-19, **2007**.
19. **V.A. Harmandaris** "Coarse graining simulations of polymers: II) Dynamics and biological applications", Proceedings, *Workshop on Mathematical and Computational Methods for Accelerated Molecular, Stochastic and Hybrid Simulation*, Heraklion, Creta, Greece, June 25-27, **2007**.
20. **V.A. Harmandaris** "Coarse graining simulations of polymers: I) Methods and applications", Proceedings, *Workshop on Mathematical and Computational Methods for Accelerated Molecular, Stochastic and Hybrid Simulation*, Heraklion, Creta, Greece, June 25-27, **2007**.
21. **V.A. Harmandaris,** M. Deserno, "Studying the Curvature Elasticity of biomembranes through numerical simulations", Proceedings, *German Physical Society (DPG)*, Dresden, Germany, March 27 – 31, **2007**.
22. **V.A. Harmandaris,** M. Deserno. "A novel method for measuring the bending rigidity of model lipid membranes by simulating tethers", Proceedings, *4th International Workshop on non-Equilibrium Thermodynamics and Complex Fluids*, Rhodes, Greece, September 3-7, **2006**.
23. **V.A. Harmandaris**, N.F.A. van der Vegt, K. Kremer "Hierarchical modeling of PS: From atomistic to coarse-grained simulations", Proceedings, *4th International Workshop on non-Equilibrium Thermodynamics and Complex Fluids*, Rhodes, Greece, September 3-7, **2006**.
24. **V.A. Harmandaris,** M. Deserno, "Studying the curvature elasticity of biomembranes through numerical simulations", Proceedings, *German Physical Society (DPG)*, Dresden, Germany, March 27 – 31, **2006**.
25. **V.A. Harmandaris,** "Polymer dynamics at interfaces: What atomistic simulations can tell us", Proceedings, *Jülich Soft Matter Days 2005*, Bonn, Germany, November 01 – 04, **2005.**
26. **V.A. Harmandaris,** K. Daoulas, V.G. Mavrantzas, "Dynamics of thin polymer melt films near at a solid attractive surface through atomistic molecular dynamics simulations", Proceedings, *European Polymer Congress 2005*, Moscow, Russia, June 26 – July 1, **2005.**
27. **V.A. Harmandaris,** K. Daoulas, V.G. Mavrantzas, "Atomistic Simulation of the Structure and Dynamics of the Polyethylene/graphite Interface", Proceedings, *3rd International Conference for Computational Modeling and Simulation of Materials (CIMTEC)*, Acireale, Italy, May 30 – June 4, **2004.**
28. **V.A. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Molecular dynamics simulation of the viscoelastic properties of long polymer melts: From Rouse to reptation theory", Proceedings, *AIChE Annual Meeting*, San Francisco, November 16-21, **2003.**
29. **V.A. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Molecular dynamics simulation of the viscoelastic properties of linear polymer melts", Proceedings, *Polymer Processing Society (PPS)*, Athens, September 14-17, **2003**.
30. **V.A. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Prediction of the viscoelastic properties of polymer from detailed molecular dynamics simulations and comparison against rheological measurements", Proceedings, *3rd Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean (EMCC-3)*, Thessaloniki, Greece, May 13-15, **2003.**
31. K. Daoulas, V.G. Mavrantzas, **V.A. Harmandaris,** A. Foteinopoulou, D.N. Theodorou, "Atomistic Monte Carlo simulations and SCF calculations of polymers at interfaces", Proceedings, *4th GRACM Congress on Computational Mechanics*, Patras, Greece, June 27-29, **2002**.
32. V.G. Mavrantzas, **V.A. Harmandaris,** D.N. Theodorou, "Hierarchical modeling of the viscoelasticity of linear polymer melts", Proceedings, *4th GRACM Congress on Computational Mechanics*, Patras, Greece, June 27-29, **2002**.
33. **V.A. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Prediction of the viscoelastic properties of high-molecular weight polymer melts through molecular dynamics atomistic simulations", Proceedings, *3rd Panhellenic Chemical Engineers' Conference*, Athens, Greece, May 31-June 02, **2001**.
34. **V.A. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Rheological properties of polymer melts from molecular constitution", Proceedings, *AIChE Annual Meeting*, Los Angeles, November 13-17, **2000.**
35. **V.A. 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", Proceedings, *XIII International Congress on Rheology*, Cambridge, UK, August 20-25, **2000**".
36. **V.A. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Atomistic modeling of viscoelastic Properties: Simulation of stress relaxation upon cessation of steady-state elongational flow", Proceedings, *International George Papatheodorou Symposium*, Patras, Greece, September 16-18, **1999.**
37. **V.A. Harmandaris,** V.G. Mavrantzas, D.N. Theodorou, "Atomistic simulation of the stress relaxation

experiment after cessation of steady-state uniaxial elongation", Proceedings, *2nd Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 27-29, **1999**.

38. V.G. Mavrantzas, **V.A. Harmandaris,** D.N. Theodorou, "Atomistic simulation of the viscoelasticity of linear polyethylene melts", Proceedings, *1st Hellenic Society of Rheology Meeting*, Heraklion, Greece, August 29-September 2, **1998**.
39. **V.A. 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**.

Presentations

1. **V.A. Harmandaris**, "Polymer/graphene systems through atomistic simulations", *9th Hellenic Polymer Society Conference"*, Salonika, Greece, November 29 – December 1, **2012**.
2. K. Johnston, **V.A. Harmandaris**, "Multi-scale modeling of polystyrene between gold surfaces", *9th Hellenic Polymer Society Conference"*, (Poster) Salonika, Greece, November 29 – December 1, **2012**.
3. **V.A. 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**.
4. **V.A. 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**.
5. **V.A. Harmandaris**, "Properties of polystyrene/graphene systems through detailed atomistic simulations", *Soft Comp Annual Meeting*, heraklion, Greece, May 10-13, **2012**.
6. **V.A. Harmandaris**, "Multi-scale simulations of fluid/solid hybrid composite systems", *18th International Conference on composite materials*, Busan, Jeju Island, Korea, August, 20-26, **2011**.
7. **V.A. 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**.
8. **V.A. 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**.
9. **V.A. Harmandaris**, "Polymer/solid interfaces through multi-scale simulations", *17th Conference on Composite Materials, ICCM*, Edinburgh, Scotland, July 27-31, **2009**.
10. **V.A. Harmandaris**, "Dynamics of entangled polystyrene through hierarchical multi-scale simulations", *7th Hellenic Polymer Conference*, Ioannina, Greece, September 28-Octomber 01, **2008**.
11. **V.A. 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.**
12. D. Fritz, **V.A. 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.**
13. **V.A. Harmandaris,** N.F.A. van der Vegt, K. Kremer "Comparing CG models: polystyrene", (Poster) *International Soft Matter Days*, Aachen, Germany, October 1-4, **2007.**
14. **V.A. Harmandaris,** M. Deserno, "Studying the curvature elasticity of biomembranes through numerical simulations", (Poster) *International Soft Matter Days*, Aachen, Germany, October 1-4, **2007.**
15. **V.A. 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.**
16. **V.A. Harmandaris,** M. Deserno, "Curvature elasticity of tethers", *Meeting of the German Physical Society (DPG) 2007*, Dresden, Germany, March 27 – 31, **2007.**
17. **V.A. 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.**
18. **V.A. 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.**
19. **V.A. 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**.
20. **V.A. 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.**

21. **V.A. Harmandaris,** K. Daoulas, V.G. Mavrantzas, "Polyethylene dynamics in polyethylene/graphite interfaces", *European Polymer Conference 2005*, Moscow, Russia, June 26 – July 1, **2005.**
22. **V.A. 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.**
23. **V.A. 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.**
24. **V.A. 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.**
25. **V.A. 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**.
26. **V.A. 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.**
27. **V.A. 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.**
28. **V.A. 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**.
29. **V.A. 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**.
30. **V.A 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**.
31. **V.A. 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**.
32. **V.A. 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**.

Invited Presentations

33. **V.A. Harmandaris**, "Molecular Simulations of Biomolecular Systems", *ACMAC workshop on "Cell biology and physiology: PDE models"*, ACMAC Center, Heraklion, Crete, Greece, October 4-6, **2012**.
34. **V.A. 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**.
35. **V.A. 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**.
36. **V.A. 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**.
37. **V.A. Harmandaris**, "Multi-scale molecular simulations of polymer interfaces", *IMPRS Workshop on "Characterization of polymer interfaces/surfaces/thin films"*, Wittenberg, Germany, April 23-27, **2012**.
38. **V.A. 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**.
39. **V.A. 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**.
40. **V.A. Harmandaris**, "Hierarchical multi-scale modeling of soft matter", *Colloquium, Department of Materials*, University of Crete, Greece, May 14, **2010**.
41. **V.A. Harmandaris**, "Molecular friction in polymers studied by multiscale simulations", *CECAM/ACAM Workshop on Molecular Friction, Dublin*, Ireland, December 14-16, **2009**.
42. **V.A. Harmandaris**, "Quantitative predictions of polymer dynamics at multiple length and time scales",

Mainz Simulation Days, Mainz, Germany, June 3-5, **2009**.

43. **V.A. Harmandaris** "Modeling of polymers: Methods and applications", *Max Planck Institute for Mathematics in the Sciences*, Leipzig, Germany, March 17, **2008**.
44. **V.A. Harmandaris**, "Multi-scale dynamic modeling of polymer and biopolymers", *Université Catholique de Louvain , Louvain-la-Neuve*, Belgium, October 12-14, **2008**.
45. **V.A. 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**.
46. **V.A. Harmandaris** "Dynamics of polymer melts in polymer/solid interfacial systems", DECHEMA, Frankfurt, Germany, June 13, **2008**.
47. **V.A. 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**.
48. **V.A. Harmandaris** "Hierarchical modeling of polymer and biopolymers", *Eindhoven University of Technology, Department of Applied Physics*, Holland, November 06, **2007**.
49. **V.A. 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**.
50. **V.A. 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**.
51. **V.A. Harmandaris** "Mesoscopic simulations of polymers and biopolymers", *Institute of Solid State Research (IFF), Theoretical Soft-Matter and Biophysics*, Jülich, Germany, February 21, **2006**.
52. **V.A. Harmandaris** "Polymer dynamics at interfaces: what atomistic simulations can tell us", *Jülich Soft Matter Days 2005*, Bonn, Germany, November 01-04, **2005.**
53. **V.A. Harmandaris** "Atomistic modelling of polymer/solid interfaces", Department of Chemical Engineering, University of Twente, Holland, April **2004**.
54. **V.A. 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**.
55. **V.A. 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**.

Organizing Conferences/Workshops

1. Member of the organizing committee for the workshop "Workshop on Software Frameworks for Challenging Computational Problems", Heraklion, Greece, January 14-18, **2013**.

Grants (current)

1. DFG SPP1369, 2008–2011. Title: "Dynamics of polymer melts near solid interfaces", Principal Investigator (PI): V. Harmandaris and H. Duran. Budget of the grant: 200.000 Euro. Duration (starting/ending) dates: 07/2008 – 06/2011. Extension (starting/ending) dates: 07/2011 – 06/2014.

2. ELKE, UOC, 2011–2013, Title: "Hierarchical multi-scale modeling of polymer nanocomposites". Principal Investigator (PI): V. Harmandaris. Budget of the grant: 15.000 Euro.

3. 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.

4. GGET, Greece (THALIS), 2012–2015. Title: "Analysis, modeling and simulations of complex systems". Role: Team Leader (PI: M. Katsoulakis). Budget of the grant: 600.000 Euro.

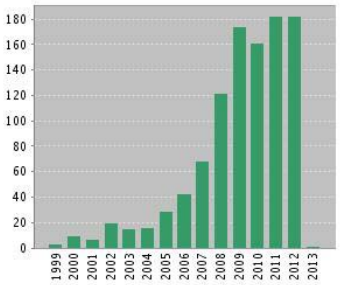
5. GGET, Greece (THALIS), 2012–2015. Title: "Self-assembly and dynamics in metastable states. From molecular and supramolecular to mesoscopic systems". Role: Team Member (PI: G. Floudas). Budget of the grant: 600.000 Euro.

6. GGET, Greece (KRHPIS), 2013–2015. Title: "Advanced – Smart Materials". Role: Team Leader. Budget of the grant: 1.573.000 Euro.

Citations (till 31/12/2012):

Total:	1023
Self:	80
Clean:	943
h-Index:	17

Citations in Each Year



Teaching

Courses taught

1. "Introduction in Monte Carlo Methods", Department of Applied Mathematics, University of Crete, Spring **2012**, Spring **2013.**
2. "Introduction to *C*", Department of Applied Mathematics, University of Crete, Fall **2012**.
3. "Biological Mathematics", Department of Applied Mathematics, University of Crete, Fall **2011**.
4. "Data Structures", Department of Applied Mathematics, University of Crete, Spring **2011**.
5. "Applied Statistics", Department of Applied Mathematics, University of Crete, Spring **2010**.
6. "Parallel Programming", Department of Applied Mathematics, University of Crete, Fall **2009,** Fall **2010**.

Teach Assistant as PhD student

1. "Introduction to Fortran", Department of Chemical Engineering, University of Patras, Fall **1997, 1998, 1999.**
2. "Numerical Analysis", Department of Chemical Engineering, University of Patras, Spring **1999**.
3. "Polymers Laboratory", Department of Chemical Engineering, University of Patras, Spring **1998.**

Graduate Students Advised and Postdoctoral Scholars

Current Postdoctoral Scholars:

1. Dr. T. Rissanou
2. Dr. K. Johnston

PhD Students:

1. T. Tsourtis

Master Students:

1. A. Power

Current Diploma Students:

1. M. Panoukidou
2. M. Vathi
3. V. Apostolopoulou

Previous Postdoctoral Scholars:

1. Dr. E. Kaligiannaki (in collaboration with Prof. M. Katsoulakis, Department of Applied Mathematics, University of Crete, Greece) 2009-2011.

Degrees Awarded:

Diploma:

1. M. Gourlis
2. M. Demetzou
3. K. Koskoletos
4. E. Kakari