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## EDUCATION

- Dec. 2006–  
March 2010 **Ph.D. in ‘Computational biophysics’**, *The University of Edinburgh, School of Engineering, Institute for Materials and Processes*, Edinburgh, UK.
- Ph.D. Thesis *‘Molecular dynamics simulations of peptide-membrane interactions’*. Use of molecular modelling and simulations to study the interaction between  $\alpha$ -helical peptides and membranes by means of Molecular Dynamics (MD) and free energy calculations.  
Supervisor: Dr. L. Sarkisov.
- Sept. 2004–  
Sept. 2006 **M.Sc. in ‘Mathematical modelling in modern technologies’**, *National Technical University of Athens*, Greece, distinction, 9.1/10 (excellent).  
Application of mathematical methods and programming to biology and physics.
- M.Sc. Thesis *‘Global modelling of the gas phase in a plasma reactor.’* Programming in C/C++ of a user-friendly simulator that solved both the mass and energy balances of a given system evident in plasma processing.  
Supervisor: Dr. E. Gogolides.
- Sept. 1999–  
June 2004 **5 year Diploma in ‘Applied mathematics and physical sciences’**, *National Technical University of Athens*, Greece, 7.7/10 (very good).  
Specialization in statistics and applied mechanics.
- Diploma thesis *‘Mathematical modelling in biology and contagious diseases’*. The thesis surveyed different models proposed for biological and physiological processes, as well as models used in epidemiology.  
Supervisor: Prof. D. E. Tzanetis.

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## CURRENT APPOINTMENT AND WORK EXPERIENCE

- Sept 2012–  
present **External collaborator**, *Prof. Liedl group*, Institute of General, Inorganic and Theoretical Chemistry, University of Innsbruck, Austria.  
Collaboration with Prof. Liedl’s group in the context of the NANODRUG ITN research project funded by the European Commission, Marie Curie Actions, Seventh Framework Programme, Initial Training Network.
- July 2010–  
present **Postdoctoral researcher in ‘Molecular modeling and computer-aided drug design’ group**, *Pharmacology and Pharmaceutology Division*, Biomedical Research Foundation, Academy of Athens, Greece.  
My work focuses on the simulations of particles with biological applications ranging from nanoparticles to membranes and protein-ligand systems using Molecular Dynamics (MD) and Monte Carlo calculations. In collaboration with Dr. Z. Cournia.
- Current projects  
- The effect of nanoparticle architecture and membrane cholesterol concentration on nanoparticle-membrane interactions using coarse-grained simulations and free energy calculations.  
- Computer-aided drug design and molecular simulations of the oncogenic mutated PI3K $\alpha$ .
- March 2010–  
June 2010 **Research associate in the ‘Studies of nanoparticle-membrane interactions’**, *University of Edinburgh, Institute for Materials and Processes*, Edinburgh, UK.  
Multiscale modeling of nanoparticle-membrane association: insights through MD simulations. In collaboration with Dr. L. Sarkisov and Prof. J. P. Ramalho.
- Sept. 2005–  
Sept. 2006 **Research associate**, *Institute of Microelectronics (IMEL), NCSR ‘Demokritos’ Institute*, Athens, Greece.  
Programming in C/C++ of a user friendly simulator that solves a system of mass and energy balances evident in plasma processing. Lead investigator: Dr E. Gogolides.

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## RESEARCH INTERESTS AND CURRENT PROJECTS

- Nanoscience Design of nano-carriers with tailored functionalities for efficient and targeted drug delivery.
- Cancer Research Targeting the mutated cancerous PI3K $\alpha$  protein with small molecule inhibitors and studying the effects of mutation in the protein's structure and dynamics using MD simulations. (Prof. Efstratiadis project)
- Drug design Developing new inhibitors for the influenza A virus M2 channel through docking, MD simulations and Free Energy Perturbation calculations. (Collaboration with Prof. Kolocouris)
- Uncertainty quantification Applying advanced mathematical techniques into quantitative characterization and reduction of uncertainties in drug design and delivery systems.

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## SELECTED PUBLICATIONS

- submitted *Z. Cournia, T. Allen, I. Andricioaei et al.*  
Membrane Proteins: Environmental Effects on Structure, Function and Dynamics.
- in press *P. Gkeka, T. Evangelidis, M. Pavlaki, V. Lazani, S. Christoforidis, B. Agianian, Z. Cournia*, PLOS COMPUT. BIOL.  
Investigating the structure and dynamics of the PIK3CA Wild-Type and H1047R oncogenic mutant.
- in press *P. Gkeka, P. Angelikopoulos, L. Sarkisov, Z. Cournia.*, PLOS COMPUT. BIOL. (corresponding author).  
Partitioning of anionic, ligand-functionalized nanoparticles in cholesterol containing membranes induces ligand rearrangement and local cholesterol depletion.
- in press *P. Gkeka, A. Papafotika, S. Christoforidis, Z. Cournia.*, J. PHYS. CHEM. B  
Exploring a Non-ATP Pocket for Potential Allosteric Modulation of PI3K $\alpha$
- May 2013 *P. Gkeka, L. Sarkisov, P. Angelikopoulos*, J. PHYS. CHEM. LETT., 4, pp. 1907-1912.  
Homogeneous hydrophobic-hydrophilic surface patterns enhance permeation of nanoparticles through lipid membranes.
- Dec. 2012 *P. Gkeka, S. Eleftheratos, A. Kolocouris, and Z. Cournia*, J. CHEM. THEORY COMPUT., 9, pp. 1272-1281 .  
Free energy calculations reveal the origin of binding preference for aminoadamantane blockers of influenza A/M2TM pore.
- Nov. 2012 *P. Gkeka, E. Athanasiadis, G. Spyrou, and Z. Cournia*, 12TH IEEE INTERNATIONAL CONFERENCE ON BIOINFORMATICS AND BIOENGINEERING  
Enhancing the effectiveness of virtual screening by using the ChemBioServer: Application to the discovery of PI3K $\alpha$  inhibitors.
- Aug. 2011 *P. Gkeka and P. Angelikopoulos*, CURRENT NANOSCIENCE, 7 (5), pp. 690-698.  
The role of patterned hydrophilic domains in nanoparticle-membrane interactions.
- March 2011 *J. P. Prates Ramalho, P. Gkeka and L. Sarkisov*, LANGMUIR, 27, pp. 3723-3730.  
Structure and phase transformations of DPPC lipid bilayers in the presence of nanoparticles: insights from coarse-grained molecular dynamics simulations.
- Jan. 2010 *P. Gkeka and L. Sarkisov*, J. PHYS. CHEM. B., 114 (2), pp. 826-839.  
Interactions of Phospholipid bilayers with several classes of amphiphilic  $\alpha$ -helical peptides: Insights from coarse-grained molecular dynamics simulations.
- Jan. 2009 *P. Gkeka and L. Sarkisov*, J. PHYS. CHEM. B., 113 (1), pp. 6-8.  
Spontaneous formation of a barrel-stave pore in a coarse-grained model of the synthetic LS3 peptide and a DPPC lipid bilayer.

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## COMPUTER SKILLS

Operating Systems	Linux, All Microsoft <sup>TM</sup> operating systems, UNIX, MacOS <sup>TM</sup> .
Programming Languages	C/C++, Fortran, shell scripting, HTML.
Scientific Tools	GROMACS, NAMD, Schrodinger, Desmond, MCPRO, VMD, Pymol, Gnuplot, MATLAB <sup>TM</sup> , Mathematica <sup>®</sup> , Comsol Multiphysics, Minitab <sup>®</sup> .
Office Automation	L <sup>A</sup> T <sub>E</sub> X, Microsoft Office <sup>TM</sup> .

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## SELECTED CONFERENCES AND INVITED TALKS

- July. 2014 NANODRUG FP7 ITN MEETING, COIMBRA UNIVERSITY, PORTUGAL. (Invited speaker)  
*The effect of membrane composition on nanoparticle-membrane interactions.*
- June. 2014 WORKSHOP ON BIOMATERIALS AND THEIR INTERACTIONS WITH BIOLOGICAL AND MODEL MEMBRANES, SALOU, SPAIN.  
*Partitioning of anionic nanoparticles in cholesterol-containing membranes.* (Oral presentation)
- Sept. 2013 CECAM WORKSHOP: COUPLING BETWEEN PROTEIN, WATER, AND LIPID DYNAMICS IN COMPLEX BIOLOGICAL SYSTEMS: THEORY AND EXPERIMENTS. (1st Poster Prize)  
*Studying the Influence of Cholesterol on Nanoparticle Partitioning into Lipid Membranes.* (Oral and Poster presentation)
- July 2013 COMPUTER-AIDED DRUG DESIGN GORDON RESEARCH CONFERENCE, WEST DOVER, VT, USA. (GRC Award)  
*Studying the influence of cholesterol on nanoparticle partitioning into lipid membranes.* (Poster presentation)
- Feb. 2013 57TH BIOPHYSICAL SOCIETY MEETING, PHILADELPHIA, USA. (CPOW Award)  
*- Study of nanoparticle-lipid bilayer interactions: insights from coarse-grained molecular dynamics simulations.*
- Nov. 2012 FACULTY OF CHEMISTRY AND PHARMACY, UNIVERSITY OF INNSBRUCK, AUSTRIA.  
*Molecular simulations of biological systems.* (Invited speaker)
- Nov. 2011 INSTITUTE OF MATERIALS AND PROCESSES MEETINGS, SCHOOL OF ENGINEERING, UNIVERSITY OF EDINBURGH, UK.  
*Molecular simulations of peptide and nanoparticle-membrane interactions.* (Invited speaker)
- Sept. 2011 THERMODYNAMICS 2011, ATHENS, GREECE.  
*The effect of hydrophobicity on nanoparticle-lipid bilayer interactions: insights from molecular dynamics and free energy calculations.* (Oral presentation)
- July 2011 STATISTICAL THERMODYNAMICS & MACROMOLECULES GROUP SEMINARS, DEPARTMENT OF CHEMICAL ENGINEERING, UNIVERSITY OF PATRAS, GREECE.  
*Molecular dynamics studies of peptide-membrane and nanoparticle-membrane interactions: insights from coarse-grained models.* (Invited speaker)
- May 2010 STRUCTURAL BIOINFORMATICS & COMPUTATIONAL BIOCHEMISTRY GROUP SEMINARS, UNIVERSITY OF OXFORD, UK.  
*Molecular dynamics studies of peptide-membrane interactions: Insights from coarse-grained models.* (Invited speaker)
- Sept. 2008 CCP5 ANNUAL MEETING: SURFACES AND INTERFACES, LONDON, UK.  
*Coarse-grained modelling of membrane-peptide interactions.* (Oral presentation)

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## GRANTS - AWARDS - SCHOLARSHIPS

- PRACE 200,000 CPU hours awarded by PRACE as the Principal Investigator (May 2014).
- Bursary Financial support from EU FP7 ITN Network to attend the NANODRUG Meeting (July 2014).
- Award 1st poster at the CECAM Workshop: Coupling between protein, water, and lipid dynamics in complex biological systems (Sept. 2013).
- Award GRC travel award to attend the Computer-aided Drug Design Gordon Research Conference (July 2013).
- Award CPOW travel award to attend the 57th Biophysical Society Meeting (Feb. 2013).
- Grant co-PI in the SYNERGASIA II grant entitled: "Magnetic Nanoparticles for targeted MRI therapy" (Jan 2013).
- Award Travel grant to attend the LinkSCEEM/Cy-Tera GPU workshop (Dec. 2012).
- Bursary Financial support to attend the CECAM Coarse-Grained Biomolecular Modeling (Oct. 2011).
- Bursary Financial support from the Bettencourt Schueller Foundation to attend the Paris Interdisciplinary PhD Symposium (June 2011).
- Scholarship 3-year scholarship and fee coverage by the Institute for Materials and Processes, University of Edinburgh, UK (Dec. 2006-Feb. 2010).
- Bursary Financial support to attend the Psi-k Summer School on 'Simulation Approaches to Problems in Molecular and Cellular Biology' provided by ESF and CECAM (Aug. 2009).
- Travel fund Travel bursary to attend FD144 Discussion 'Multiscale Modelling of Soft Matter' from Royal Society of Chemistry (July 2009).
- Bursary Bursary to attend the workshop 'Understanding Molecular Simulations' provided by Marie Curie Actions-MolSimu and CECAM (Jan. 2007).
- Scholarship Award by State Scholarships Foundation of Greece for fulfilling my M.Sc. studies with first distinction (June 2006).
- Travel fund Expenses covered by the European Commission grant to participate to the European Conference on Mathematical and Theoretical Biology (ECMTB) (July 2005).
- Travel fund Bursary to attend 'Euroschola', Strasbourg, France, representing Greece after an essay competition on the 'Effects of the Maastricht treaty in Greece' (March 1998).

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## LANGUAGES

Greek	Mother tongue	(Native language)
English	Fluent	(Cambridge Certificate of Proficiency in English (CPE))
French	Very good knowledge	(La Sorbonne II)
Spanish	Beginners	(Some knowledge)
Portuguese	Beginners	(Some knowledge)