Curriculum Vitae

Personal Data

First Name:	Anthony
Last name:	Chazirakis
Date of Birth:	29th of March 1976
Place of Birth:	Chania – Crete - Greece
e-mail:	thazir@gmail.com

Studies

- **PhD on "Multi-scale Modeling of Macromolecular Systems via Physics-based Data-driven Models" at the Department of Applied Mathematics of the University of Crete**
  (*with strong focus on HPC software development, setup and administration)*
- **Masters Degree on "Scientific Computing" at the Department of Applied Mathematics of the University of Crete**
  (*with strong focus on HPC software development, setup and administration, thesis on "Stochastic and Deterministic Parametrization of Coarse Graining models for Molecular Systems"*)
- **Bachelor's Degree on Physics at the Department of Physics of the University of Crete**
  (grade 7.41 out of 10, thesis on "Parallel Molecular Dynamics Simulations")
- **Cambridge First Certificate of English Language**
  (very fluent, many years of practice in studying technical documents, ease at writing technical documents)

Post Doc Experience

- Post doctoral research associate at IACM, FORTH.
  - From 11 Sep 2025 to 31 Dec 2025 at the «THUNDER 15515 ELIDEK ΑΠ 80196/18-1-24» project.
  - From 1 Jan 2026 till today at the «TOYOTA MOTOR COPRORATION» project.
  - Research topic: Molecular Simulations and Machine Learning Models of Complex Polymer Nanocomposites.

Research Interests

- Molecular Dynamics Simulations
- Coarse Graining of Molecular Systems
- Machine Learning Models for the Coarse Graining of Molecular Systems
- Numerical Optimization Methods

- Atomistic Detail Back-Insertion
- Parallel and High Performance Scientific Computing

General

I chose to study Physics out of genuine interest. Although I have had significant successes at the beginning of my studies I had to quit due to financial difficulties. I started working as a software developer and IT technician and kept doing so for many years. Much later I had the will and opportunity to complete my studies achieving a fairly good grade. During my studies I focused on computational courses. I have also applied for a master's degree on the subject and have completed my postgraduate studies on scientific computing.

Since the beginning of my postgraduate studies, with a small break during 2016 to 2017, I have been working for various research institutes at Heraklion of Crete. My work mostly involves the development of HPC computational algorithms at the field of molecular dynamics and of coarse graining of molecular systems. Aside from others, I have coded a hybrid parallel molecular dynamics simulatior in C++, with MPI and OpenMP, a coarse graining toolkit using the Iterative Boltzmann Inversion method in Python and a package of molecular dynamic post processing tools in mixed Python with C++ and OpenMP. Furthermore I have set up HPC computational resources of the order of 200 cpus for the research group I am part of and I provide administrative and general IT support services for them.

I started my PhD in July 2019 and I successfully presented my thesis on the second of June 2025. I focused in exploring various methods for the coarse graining of molecular systems, including machine learning methods for the task. I have received a scholarship funded from the “Goodyear Tire and Rubber Company” and worked on the coarse graining and analysis of rubber polymers. During my PhD I continued to work on and evolve the HPC codes I have already implemented.

After the completion of my PhD I have been working as post doctoral research associate at IACM, FORTH, from 11 Sep 2025 to 31 Dec 2025 at the «THUNDER 15515 ELIDEK ΑΠ 80196/18-1-24» project and from 1 Jan 2026 till today at the «TOYOTA MOTOR COPRORATION» project. My research topic is “Molecular Simulations and Machine Learning Models of Complex Polymer Nanocomposites”.

Overall, I have collaborated with several researchers, providing the computational tools needed for the calculations involved at several publications. I work mostly with Python, Numba and Mpi4Py in order to quickly produce efficient code. I have accumulated significant experience at high performance scientific computing and the development of parallel algorithms focused around the field of molecular dynamics simulations. Throughout my studies I have acquired the necessary theoretical background in molecular dynamics, statistical mechanics and numerical analysis, so as to be able to collaborate with researchers seeking programmatic support. I have contributed to twenty publications, performing scientific computing work.

Published Papers

1. Malak Barakat, Anthony Chazirakis, Vagelis Harmandaris, Hilal Reda “Fracture behavior of immiscible polymer blends: A combined atomistic-continuum simulation approach”, Engineering Fracture Mechanics, Volume 345, Part A, 2026, 112353, https://doi.org/10.1016/j.engfracmech.2026.112353

2. Rohit Ghanta, Anthony Chazirakis, Craig Burkhart, George Papakonstantopoulos, Patrycja Polinska, Vagelis Harmandaris, Manolis Doxastakis, “Modeling chain relaxation in moderately entangled polyisoprene melts”, *Macromolecules* (2025) 58 (23): 12893–12908, https://doi.org/10.1021/acs.macromol.5c02521.

3. Spyros V. Kallivokas, Anthony Chazirakis, Rohit Ghanta, Anastassia Rissanou, Patrycja Polińska, Craig Burkhart, Manolis Doxastakis and Vagelis Harmandaris, “Elastic, viscoelastic, dynamic, topological and structural properties of crosslinked SBR through atomistic molecular dynamics simulations”, Soft Matter, 2025,21, 5743-5751, https://doi.org/10.1039/d5sm00126a.

4. Hilal Reda, Panayiota Katsamba, Anthony Chazirakis, Vagelis Harmandaris, “Revealing the Role of Microstructure and Strain Heterogeneities in the Elastic–Plastic Transition of Glassy Polymers”, Macromolecules 2025, 58, 14, 6994–7004, https://doi.org/10.1021/acs.macromol.5c00694.
(implementations in mpi4py and numba)

5. H. Reda, P. Katsamba, A. Chazirakis, and V. Harmandaris, “Probing the Linear-to-Plastic Transition in Polymer Nanocomposites via Atomistic Simulations: The Role of Interphases,” *Macromol. Rapid Commun.*, p. 2400612, 2024, https://doi.org/10.1002/marc.202400612.
(implementations in mpi4py and numba)

6. H. Reda, A. Chazirakis, A. F. Behbahani, N. Savva, and V. Harmandaris, “Revealing the Role of Chain Conformations on the Origin of the Mechanical Reinforcement in Glassy Polymer Nanocomposites,” *Nano Lett.* 10 January 2024; 24 (1): 148–155, https://doi.org/10.1021/acs.nanolett.3c03491.
(implementations in mpi4py and numba)

7. M. Barakat, H. Reda, A. Chazirakis, and V. Harmandaris, “Investigating the mechanical performance of graphene reinforced polymer nanocomposites via atomistic and continuum simulation approaches,” *Polymer (Guildf).*, vol. 286, p. 126379, 2023, https://doi.org/10.1016/j.polymer.2023.126379.
(implementations in mpi4py and numba)

8. I. Tanis, A. J. Power, A. Chazirakis, and V. A. Harmandaris, “Heterogeneous glass transition behavior of poly (ethylene oxide)/silica nanocomposites via atomistic MD simulations,” *Macromolecules*, vol. 56, no. 14, pp. 5482–5489, 2023, https://doi.org/10.1021/acs.macromol.3c00593.

9. H. Reda, A. Chazirakis, N. Savva, J.-F. Ganghoffer, and V. Harmandaris, “Gradient of mechanical properties in polymer nanocomposites: From atomistic scale to the strain gradient effective continuum,” *Int. J. Solids Struct.*, vol. 256, p. 111977, 2022, https://doi.org/10.1016/j.ijsolstr.2022.111977.
(implementations in mpi4py and numba)

10. *Eleftherios Christofi*, *Antonis Chazirakis*, *Charalambos Chrysostomou*, *Mihalis A Nicolaou*, *Wei Li*, *Manolis Doxastakis*, *Vagelis A Harmandaris*, “Deep convolutional neural networks for generating atomistic configurations of multi-component macromolecules from coarse-grained models,” *J. Chem. Phys.*, vol. 157, no. 18, 2022, https://doi.org/10.1063/5.0110322.

11. H. Reda, A. Chazirakis, A. J. Power, and V. Harmandaris, “Mechanical behavior of polymer nanocomposites via atomistic simulations: conformational heterogeneity and the role of strain rate,” *J. Phys. Chem. B*, vol. 126, no. 38, pp. 7429–7444, 2022, https://doi.org/10.1021/acs.jpcb.2c04597.

12. H. Reda, A. Chazirakis, A. F. Behbahani, N. Savva, and V. Harmandaris, “Mechanical properties of glassy polymer nanocomposites via atomistic and continuum models: The role of interphases,” *Comput. Methods*

Appl. Mech. Eng., vol. 395, p. 114905, 2022, https://doi.org/10.1016/j.cma.2022.114905.
(implementations in mpi4py and numba)

13. H. Reda, A. Chazirakis, A. F. Behbahani, N. Savva, and V. Harmandaris, "A methodology for determining the local mechanical properties of model atomistic glassy polymeric nanostructured materials," *MethodsX*, vol. 9, p. 101931, 2022, https://doi.org/10.1016/j.mex.2022.101931.
(implementations in mpi4py and numba)

14. A. Rissanou, A. Chazirakis, P. Polinska, C. Burkhart, M. Doxastakis, and V. Harmandaris, "Polybutadiene copolymers via atomistic and systematic coarse-grained simulations," *Macromolecules*, vol. 55, no. 1, pp. 224–240, 2021, https://doi.org/10.1021/acs.macromol.1c01939.

15. Behbahani A, Schneider L, Rissanou A, Chazirakis A, Bačová P, Jana P, Li W, Doxastakis M, Polińska P, Burkhart C, Müller M, Harmandaris V, "Dynamics and rheology of polymer melts via hierarchical atomistic, coarse-grained, and slip-spring simulations," *Macromolecules*, vol. 54, no. 6, pp. 2740–2762, 2021, https://doi.org/10.1021/acs.macromol.0c02583.

16. T. Jin, A. Chazirakis, E. Kalligiannaki, V. Harmandaris, and M. A. Katsoulakis, "Data-driven Uncertainty Quantification for Systematic Coarse-grained Models," *Soft Mater.*, pp. 1–21, 2020, https://doi.org/10.1080/1539445X.2020.1765803.
(parallel Matlab)

17. 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.*, vol. 152, no. 12, p. 124902, Mar. 2020, https://doi.org/10.1063/1.5143245.
(implementation of local density potentials in a custom hybrid MPI + OpenMP molecular dynamics simulator in C++)

18. G. Zhang, A. Chazirakis, V. A. Harmandaris, T. Stuehn, K. C. Daoulas, and K. Kremer, "Hierarchical modelling of polystyrene melts: from soft blobs to atomistic resolution," *Soft Matter*, vol. 15, no. 2, pp. 289–302, 2019, https://doi.org/10.1039/c8sm01830h.

19. J. Herbrych, A. G. Chazirakis, N. Christakis, and J. J. P. Veerman, "Dynamics of Locally Coupled Agents with Next Nearest Neighbor Interaction," *Differ. Equations Dyn. Syst.*, 2017, https://doi.org/10.1007/s12591-017-0377-3.
(parallelly solved a very large set of initial value problems with MPI in C++)

20. E. Kalligiannaki, A. Chazirakis, A. Tsourtis, M. A. Katsoulakis, P. Plecháč, and V. Harmandaris, "Parametrizing coarse grained models for molecular systems at equilibrium," *Eur. Phys. J. Spec. Top.*, vol. 225, no. 8, pp. 1347–1372, 2016, https://doi.org/10.1140/epjst/e2016-60145-x.
(parallel Matlab)

Programming Languages and Libraries

- Excellent knowledge of:
  C, C++, Python (also numpy, scipy, matplotlib, numba), Delphi (Pascal), SQL

- Very good knowledge of:
  MPI, OpenMP, Fortran, Matlab (also parallel)

- Good knowledge of:
  Parallel Debugging and Profiling, HTML, PHP, Qt C++ Framework, Javascript, Visual Basic, Informix New Era, Cobol

- A few implementations with:
  CUDA, Vectorization Pragmas, C#, Java, Shell Scripting in Linux and Windows (PowerShell), Flash ActionScript, Joomla Framework, Mathematica

Development Environments and Tools

- Excellent knowledge of:
  Visual Studio Code (Python/C++), Codegear RAD Studio (Delphi), Microsoft Visual Studio (C++, Fortran, C#), MySql (DB), Firebird (DB), Office Applications (*Word*, *Excel*, *PowerPoint*, *Access*, *etc)*

- Good knowledge of:
  Eclipse (C++, Fortran), Qt Creator (C++), Informix (Database),

- A few implementations with:
  MS SQL (Database), Macromedia Flash

Operating Systems

- Excellent knowledge of Windows.

- Very good knowledge of Linux.

- Basic knowledge of HPC Cluster setup.

Non-Professional Experience

PhD Thesis

In English, “Multi-scale Modeling of Macromolecular Systems via Physics-based Data-driven Models”. Coarse graining methodologies and toolkit for simple and complex molecular systems. Study of transferability of coarse grained industrial rubber model. Evaluation of local density depended coarse grained model for polyisoprene. Reinsertion of atomistic details at coarse grained systems. Bridging of the atomistic and continuum scales through the study of the mechanical properties polymer-nanoparticle composite systems. Experimentation with data-driven machine learning methods for the coarse graining of molecular systems. Parallel implementations in Matlab, C++ and Python.

Master's Thesis

In English, *“Stochastic and Deterministic Parametrization of Coarse Graining models for Molecular Systems”*. A comparative study of the “Force Matching”, “Iterative Boltzmann Inversion” and the “Relative Entropy” Coarse

Graining methods on liquid Methane. Parallel implementations in Matlab, C++ and Python. Stochastic and Deterministic linear and non linear optimization methods.

Bachelor's Thesis

In English, *"Parallel Molecular Dynamics Simulation in C++"*. Hybrid MPI-OpenMP implementation in C++. Later addition of CUDA. Simulation of complex molecular systems with the classical approach of molecular mechanics. Work on HPC cluster for more than one year for development, optimization, and profiling of the simulation using tools like VampirTrace and MPE.

Workshops

Workshop on Accelerated High-Performance Computing in Computational Sciences, International Centre for Theoretical Physics, Trieste, Italy, 25 May to 5 June 2015, on the topics of GPU optimizations with CUDA and CPU optimizations with OpenMP and vectorization.

Classes

I have been successfully taught Fortran, C, C++, Java, Computational Physics, Parallel Programming, Numerical Analysis, Monte Carlo Methods, Statistical Physics and Classical Mechanics.

Professional Experience

Computing in General

- I have full twenty years of experience in software development for office database applications, using multiple programming languages and tools. During that time i also offered IT support and services to home and small office users as well as government agencies. I am still involved in such work, but to a much lesser extent. I am mostly focused to a few medical professionals and government agencies.

Scientific Computing

- Since November 2017 till today. I have been working for the Institute of Applied and Computational Mathematics at FORTH. I have coded in Python, mostly, a Molecular Dynamics Coarse Graining toolkit that automates the execution and data analysis of simulations, in order to implement well known Coarse Graining methodologies for generic molecular systems. Some machine learning methods for coarse graining molecular systems have been investigated, using neural networks and kernel based methods. I have coded a multitude of analysis tools for molecular dynamics simulations, while performing the analysis of rubber polymer systems. For almost the past year I have been working as a post doctoral research associate on the topic of "Molecular Simulations and Machine Learning Models of Complex Polymer Nanocomposites". I have been also been providing IT support and cluster administration services throughout the years.

- August to September 2020: Internship at "Computation-based Science and Technology Research Center" of "The Cyprus Insitute" at Cyprus. Development of a web site for the presentation of the results of some models of spreading of COVID-19.

- February 2016. Extension of work previously done for the School of Biological and Chemical Sciences of Queen Mary's University of London with Dr. Aristides Moustakas. Extension of the model to include brumbles, the primary food source of Deer, and the effects of rainfall and temperature levels over the years.

- During 2014 and 2015. I have been working as an associate for the Department of Applied Mathematics of the University of Crete and then for the Institute of Applied Mathematics at FORTH. Specifically I have been working for professor Vagelis Harmandaris, continuing the development of the molecular dynamics simulation package I started my bachelor's thesis on.

- From the middle of April 2014 until November 2014 i worked as an associate of the School of Biological and Chemical Sciences of Queen Mary's University of London. I participated at work assigned by the postdoctoral research assistant Aristides Moustakas, under the subject “Model Development In Computational Ecology Using An Agent Based Model”. Specifically I was assigned to check the correctness of an existing forest simulation code in C++ and to extend it adding an interacting deer model to it.

- During 2005. I rewrote the Skinakas Observatory telescope autoguider, which I converted from C and DOS to Delphi and Windows.

- During 1995. I converted existing code from Fortran to C for the Drosophila Genome Mapping project of IMBB-Forth. I worked in Windows and VMS.

Non Scientific Computing

The list is non exhaustive but indicative of the works performed. The dates are of medium accuracy. These works are usually accompanied by the support and maintenance of the customer systems and of periodic software upgrades.

- 2019 till today: Occasional upgrade of already deployed software and frequent technical support and administration on Windows Server networks.

- November 2018: Upgrade of Procurement List application for NAMFI in Delphi and MySql.

- October 2018. Automation of large volume of user data backups in Linux with Python and Rsync. Fair distribution of available storage space among users. Prioritization of most important data from users through simple configuration files.

- September 2018: Setup of Windows 2018 servers. Usage of Virtual Machines as a plan for disaster recovery. Automated daily backups of VMS to redundant network locations. Automated daily monitoring of physical server for hardware events. Results of automated jobs are emailed to users in compact format and thus system health is monitored with minimal effort.

- During 2017. Upgrade of two previously installed medical Picture Archiving and Communications Systems. Addition of Modality Worklists to previously developed Radiology software.

- Dec 2015 - Feb 2016. Writing of two new applications for NAMFI in Delphi and MySql.

- 2014-2015. Various support and upgrades to ERP, Court management software, etc.
- 2012-2013. Rewriting of various applications for NATO Missile Firing Installation in Crete. Coding in Delphi, Qt C++ and Windows. Setup and maintenance of Windows Domain, Distributed File System with Replication, Exchange Server, Virtualized Database Server, multiple (40+) computers and users, usage of PowerShell and Python for administrative tasks.
- 2011. Creation of website for the Chania Lawyers Bar in Joomla and PHP – MySql. Also various updates of the previously written by me desktop office application.
- 2009-2010. Writing of software for court data management for the courts of Chania, Thrace and Heraklion in Delphi and Windows.
- 2008. Writing of ERP software in Delphi and Windows. Writing of accompanying software for Windows Pocket Pc in C#. Multiple customers.
- 2007. Web site development for Cayo Beach Bar in Flash and ActionScript.
- 1998-2001. Development of multiple applications with Informix New Era for the NATO Missile Firing Installation in Crete. Installation and administration of an Informix Database Server in a Windows Domain.
- 1993. Participation at the development and support of ERP like software written with Cobol and working on DOS, Windows and SCO Unix.