HELLENIC REPUBLIC
MINISTRY OF EDUCATION AND RESEARCH
GENERAL SECRETARIAT FOR RESEARCH AND TECHNOLOGY

FOUNDATION FOR RESEARCH AND TECHNOLOGY – HELLAS
INSTITUTE OF APPLIED AND COMPUTATIONAL MATHEMATICS

One Post-doctoral Research Fellow at IACM/FORTH on

Computational Modeling and Machine-Learning Algorithms for Polymeric Materials

Job Description

A post-doctoral research position in the field of computational modeling across scales and machine learning algorithms for polymeric materials is available at the Institute of Applied and Computational Mathematics (IACM), of the Foundation for Research and Technology Hellas (FORTH) (group of Prof. V. Harmandaris).

The applicant will be responsible for designing and performing hybrid computational approaches combining molecular simulations and ML techniques, for a variety of model systems, related to the development of modern advanced elastomers used in the rubber industry. The methods will be designed using first principles or reference experiments and will provide the local morphology and dynamics of macromolecules with and without fillers as a function of composition. To cover a wide range of temperatures and compositions efficiently, high-fidelity transferable coarse-grain models need to be developed and modeled. Results from these simulations will serve as input to available mesoscopic modeling providing means for targeted design of high-performance elastomers [1-4].

We are seeking qualified applicants with a Ph.D. in Applied Mathematics, Engineering, Materials Science, Chemistry or Physics with strong skills and experience with molecular simulations of polymers including coarse-graining techniques. Research productivity in the form of presentations and publications is expected. The candidate should also have good personal skills for working in a team environment.

The project is part of a collaboration with the *Goodyear Tire & Rubber Company*, *University of Goettingen*, Germany and *The University of Tennessee*, Knoxville, USA. The candidate will contribute as part of a team of researchers working in concert to enable and execute new research thrusts with specific aims and deliverables as identified in the project. FORTH is a major research organization in Greece, with the mission to pursue high quality basic and applied research. IACM (www.iacm.forth.gr) focuses its research activities in several fields of natural sciences and engineering, including multi-scale modelling of complex systems and computational methods, being the main applied and computational mathematics research centre in Greece.

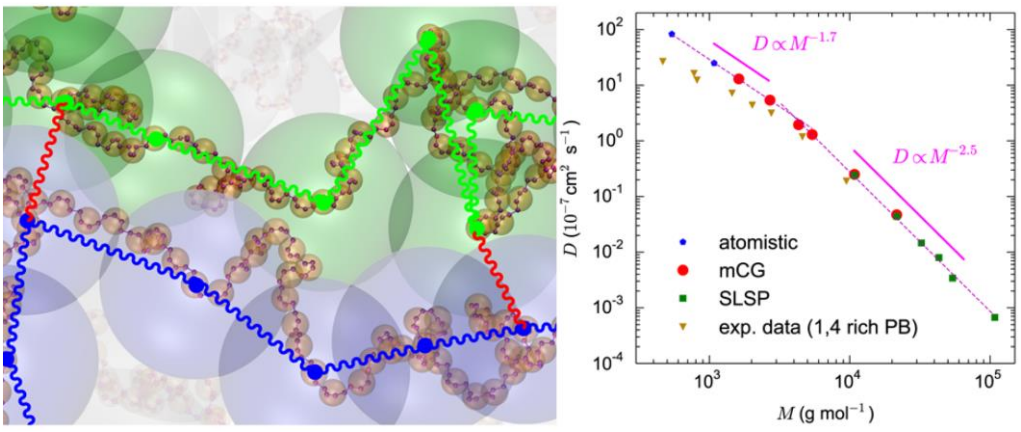

Figure: A triple scale systematic computational methodology to link atomistic, CG and mesoscopic simulation approaches for studying the dynamics and the rheology of polymeric systems [1].

The position is immediately available and the *duration is from 1 up to 3 years*. Applications received before July 30th 2022 will receive immediate attention; however, applications will be reviewed thereafter until the position is filled. Interested applicants should contact **Prof. Vagelis Harmandaris** (harman@uoc.gr). Candidates should offer a CV together with a description of their research experience and interests, including names and contact information of three references. Interested candidates who meet the aforementioned requirements are kindly asked to submit their applications to the secretariat of IACM Ms. M. Papadaki (mariapap@iacm.forth.gr).

References

1. A. F. Behbahani, et al., Macromolecules, 2021, 54, 6, 2740–2762
2. A. F. Behbahani, et al., Macromolecules, 2020, 53, 15, 6173–6189
3. W. Lei, et al., J. Chem. Phys, 2020, 153, 041101
4. A. Rissanou, et al., Macromolecules, 2022, 55, 1, 224–240.