POSTDOCTORAL FELLOWSHIP IN MULTISCALE SIMULATION OF POLYMERIC SYSTEMS AND

Company Description

BCAM is the Research Center on Applied Mathematics created with the support of the Basque Government and the University of the Basque Country, which aims to strengthen the Basque science and technology system, by performing interdisciplinary research in the frontiers of mathematics, talented scientists' training and attraction, so the excellence of our results are recognized by the Society

Information

Deadline: 2023-03-31
Category: Business
Province: Bizkaia
Country: Basque Country
City: Bilbao

Company

BCAM

Main functions, requisites & benefits

Main functions

Multiscale simulation of polymeric systems and adhesives materials

Applications are invited for a 2-years postdoctoral position in multiscale modelling of complex fluid/materials at the CFD group (BCAM). The goal is to develop a fundamental understanding of the nature of polymeric adhesives. Adhesives are complex polymeric materials that work on the basis of interactions that occur across multiple length scales. For example, in a polymeric pressure sensitive adhesive the bond between the adhesive and the substrate occurs at the molecular level but the macroscopic behaviour observed is largely the result of chain dynamics at the macromolecular level. Understanding adhesion thus requires linking phenomena occurring over multiple orders of magnitude in length and time. The group in BCAM has worked for a long time on simulation of complex fluids using mesoscopic [1] and continuum methods [2]. Very recently a fully Lagrangian Heterogeneous Multiscale Method (L-HMM) framework based on Smoothed Dissipative Particle Dynamics (SDPD) has been proposed, which allows for the integration of simulations performed at the microscopic scale to macroscopic problems with full incorporation of flow history and memory effects [3,4]. In this project, this multiscale simulation framework will be extended to the more complex phenomena of adhesion, involving simulation of contact between adhesive and substrate and
the debonding process.

The postdoctoral candidate will work under the supervision of Ikerbasque Prof. Marco Ellero (CFD group, BCAM) on modelling and HPC simulations of the above mentioned systems. The project will benefit from close collaboration with the Polymerization Processes group at POLYMAT (Prof. José María Asua: https://www.polymat.eu/en/groups/polymerization- processes-group) which has extensive experience in the development of polymeric adhesives from synthesis to macroscopic applications and possess state-of-the-art analytical techniques for a detailed structural characterization of the complex polymeric systems and adhesives.

[1] DN Simavilla, M Ellero , "Mesoscopic simulations of inertial drag enhancement and polymer migration in viscoelastic solutions flowing around a confined array of cylinders" Journal of Non-Newtonian Fluid Mechanics 305, 104811 (2022).

[2] DN Simavilla, P Español, M Ellero , "Non-affine motion and selection of slip coefficient in constitutive modeling of polymeric solutions using a mixed derivative" Journal of Rheology 67 (1), 253-267 (2023)

[3] N Moreno, M Ellero, "Arbitrary flow boundary conditions in smoothed dissipative particle dynamics: A generalized virtual rheometer" Physics of Fluids 33 (1), 012006 (2021).

[4] N Moreno, M Ellero, "Generalized Lagrangian Heterogenous Multiscale Modeling of Complex Fluids" arXiv preprint arXiv:2211.05080 (2023)

Requisites

Excellent young researchers.

Applicants must have their PhD completed before the contract starts