

Schedule of planned research work

Active polymer brushes

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Applicant: Lic. Kevin Speyer
Home institution: National Atomic Energy Commission, Pcia. Buenos Aires, Argentina
Host institution: Institut für Theoretische Physik, Georg-August Universität, Göttingen
Duration: 2 months
Starting date: May 2018

1 Schedule

- 1 May to 1 June: Channel with explicit solvent: synchronization and hydrodynamic coupling
 - An explicit solvent will be added to channel coated by active brushes, described by Lennard-Jones particles, to account for momentum conservation and the concomitant hydrodynamic interactions, taking advantage of the experience of the German group.
 - We will analyze the effect of solvent-mediated hydrodynamic coupling between active chains and characterize changes in the collective chain dynamics, as compared to the case of elastic coupling alone (in dry brushes).
- 1 June to 1 July: Liquid flow with synchronized chain dynamics
 - Imposing coordinated movement to the chains, mimicking typical cilia dynamics, we will study the flow generated in the solvent.
 - Upper and lower active brush layers of the slit channel will be studied as a function of polymer beating frequency, amplitude, and direction. Directed flow in the vicinity of the individual active brush layers can be achieved by choosing parameters that result in synchronization, or by imposing a phase-locked dynamics with a time-dependent external force.
 - Special interesting cases are in-phase movement of active upper and lower brushes and anti-phase movement of upper and lower grafted layers. If the polymers

drive locally the fluid, the in-phase movement is expected to produce a plug flow, whereas the anti-phase movement results in shear flow.

- A parallelization scheme with GPU of some parts of the code will be studied and implemented by the applicant with the help of the Prof. Müller and his group.