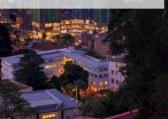
Workshop

Mechanical Forces in Biology: Theory and Simulation

September 30–October 2, 2019 Universidad de los Andes Bogotá, Colombia



SPEAKERS:



Alfredo Alexander-Katz MIT Cambridge, USA



Pilar Cossio UdeA Medellín, Colombia



Frauke Gräter HITS Heidelberg, Germany



Helmut Grubmüller MPI-BPC Göttingen, Germany



José Daniel Muñoz UNAL Bogotá, Colombia



Ulrich Schwarz Heidelberg U. Heidelberg, Germany

Organized by: Max Planck Tandem Group in Computational Biophysics at UNIANDES

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mptg-cbp.github.io/ teaching/for-biol-2019

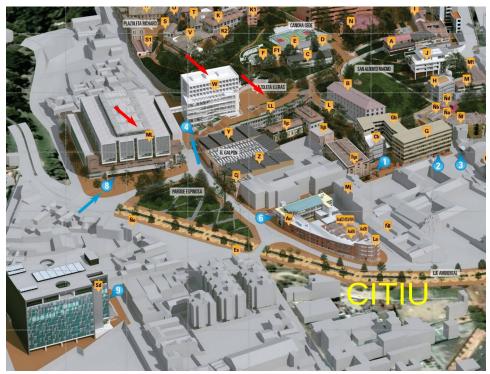
MAPS

Buildings (red arrows): W, ML, and LL

ROOM: TO BE DEFINED Entrances (blue arrows):

Entrance 4. "Lleras" Address: Calle 19A Nº 1 - 37 Este

Entrance 8. "Mario Laserna" Address: Cra. 1 Este Nº 19A - 40





PROGRAM OVERVIEW

TROOKAM OVERVIEW						
	Monday (30.09)	Tuesday (01.10)	Wed. (02.10)			
8:00 – 9:00	Registration					
9:00 – 9:30	Welcome					
9:30 – 10:30	Helmut Grubmüller	Frauke Gräter	Pilar Cossio			
10:30 - 11:00	Coffee break					
11:00 – 12:00	Frauke Gräter	Helmut Grubmüller	Alfredo Alexander- Katz			
12:00 - 14:00	Lunch					
14:00 – 15:00	Alfredo Alexander- Katz	Ulrich Schwarz	CT: Helman Amaya			
			CT: Sergio Cruz-León			
15:00 – 15:30	CT: A. Sandoval	CT: Alberto Castillo	logá D. Muñoz			
15:30 – 16:00	Coffee break	Doctor coocian	José D. Muñoz			
16:00 – 17:00	Ulrich Schwarz	Poster session	Departure			

PRESENTATION

Mechanical forces are ubiquitous in biology. At the macroscopic level, mechanical stress influences key aspects such as the morphology or the growth of tissues and organs. In addition, specific organs, like the ear, have evolved to work as highly sensitive detectors of mechanical signals. Moreover, biological frameworks, such as silk fibers, are fabulous materials, designed to withstand large mechanical stresses while staying very flexible. At the cellular level, mechanics define vital processes such as stability, division, proliferation, or migration of cells. At the molecular level, mechanical forces stimulate ion channels, molecular motors, or adhesive proteins to trigger their function. Mechanical forces are also manifested in diseases. For instance, bacteria and parasites use the shear-stress of flows to adhere more firmly to host cells.

Theoretical and simulation approaches have greatly contributed to our understanding of how biological systems cope with mechanical forces. The goal of the workshop is thus to bring a selected group of renown scientist, to provide the basis and the state of the art of mechanical forces in biology, over a wide resolution range, from biomolecules to organs, from a theoretical and a simulation perspective.

The workshop is addressed to students, researchers, and professors interested in this area. The participants will have the opportunity to interact with the invited speakers and to present their own work in contributed talks and poster presentations.

Topics include:

- Biomaterials: spider silk
- Mechanics of focal adhesions
- Mechanics of collagen fibers
- Blood clotting
- Biophysics of malaria
- Cells in shear flow
- Collective cell migration
- Molecular motors
- Ribosomal translation
- Force-probe simulations
- Modeling of the cochlea
- ...

PROGRAM IN DETAIL

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Monday, S	Septemb	er 30			
Time	Room				
8:00 – 9:00		Registration			
9:00 – 9:30		Welcome			
9:30 – 10:30		Helmut Grubmüller MPIBPC, Göttingen	Force-probe molecular dynamics simulations		
10:30 – 11:00		Coffee break			
11:00 – 12:00		Frauke Gräter HITS, Heidelberg	Mechanics of focal adhesions and collagen fibers		
12:00 – 14:00		Lunch			
14:00 – 15:00		Alfredo Alexander- Katz. MIT, Cambridge	Adsorption of soft materials under non- equilibrium conditions		
15:00 – 15:30		Contributed talk: Angélica Sandoval UNIANDES, Bogotá	The interaction of blood proteins with extracellular DNA		
15:30 – 15:40		Photo			
15:40 – 16:00		Coffee break			
16:00 – 17:00		Ulrich Schwarz U. Heidelberg	Introduction to modeling cell mechanics and adhesion		
19:00 –		Invited speakers dinner			
Tuesday, October 1					
9:30 – 10:30		Frauke Gräter HITS, Heidelberg	Spider silk and other biomaterials with exceptional mechanical properties		
10:30 – 11:00		Coffee break			
11:00 – 12:00		Helmut Grubmüller MPIBPC, Göttingen	Molecular motors & Ribosomal translation		
12:00 – 14:00		Lunch			
14:00 – 15:00		Ulrich Schwarz U. Heidelberg	Biophysics of malaria-infected red blood cells		
15:00 – 15:30		Contributed talk: Alberto Castillo	A parasite's thoughts: What is like to swim inside you?		
15:30 – 17:30		Poster session (with drinks and finger food)			

Wednesday, October 2				
9:30 – 10:30		Pilar Cossio UDEA, Medellín	Rates and transition paths in atomic force spectroscopy	
10:30 - 11:00		Coffee break		
11:00 – 12:00		Alfredo Alexander- Katz. MIT, Cambridge	biological or bio-inspired biopolymers under flows: blood clotting	
12:00 – 14:00		Lunch		
14:00 – 14:30		Contributed talk: Helman Sandoval UNIANDES, Bogotá	Dynamics of self-interacting bio-inspired polymers in shear flows	
14:30 – 15:00		Contributed talk: Sergio Cruz-León MPI-Biophysics, Frankfurt	Specific effects of metal cations in RNA: the interplay of binding affinity and kinetics	
15:00 – 16:00		José D. Muñoz UNAL, Bogotá	Modeling of the propagation of sound through the cochlea	
16:00 – 16:30		Closing remarks and departure		

POSTERS

1	Leonel Ardila UNAL, Bogotá	Heat exchange fluctuation relation in the transition between a micro-canonical and a canonical ensemble
2	Iván Pulido UNIANDES, Bogotá	Structural modeling and charge-distribution of the shear- sensitive Plasmodium falciparum adhesin VAR2CSA
3	Sebastian Ortiz UDEA, Medellín	The similarity between the probability distributions of cryo-EM reconstructions can control overfitting
4	Valeria Mejía UNIANDES, Bogotá	The effect of G1324A and G1324S mutations on the complex formed by the von Willebrand factor A1 domain and the glycoprotein lba-platelet receptor, studied through molecular dynamics simulations and free energy calculations.
5	Juan Orjuela UNIANDES, Bogotá	Effect of lipid-protein interactions on the hemostatic function of the mechanoactivated platelet glycoprotein IB membrane receptor
6	Gilles Pieffet UAN, Bogotá	Determination of the Binding Free Energy of a peptide inhibitor of the N-Methyl-D-Aspartate (NMDA) Receptor using Umbrella Sampling
7	Santiago Agudelo UDEA, Medellín	Steered molecular dynamics simulations for studying ZIKV E protein- Glycosaminoglycan interaction.