Workshop

Mechanical Forces in Biology: Theory and Simulation

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

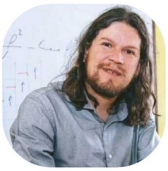
SPEAKERS:

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

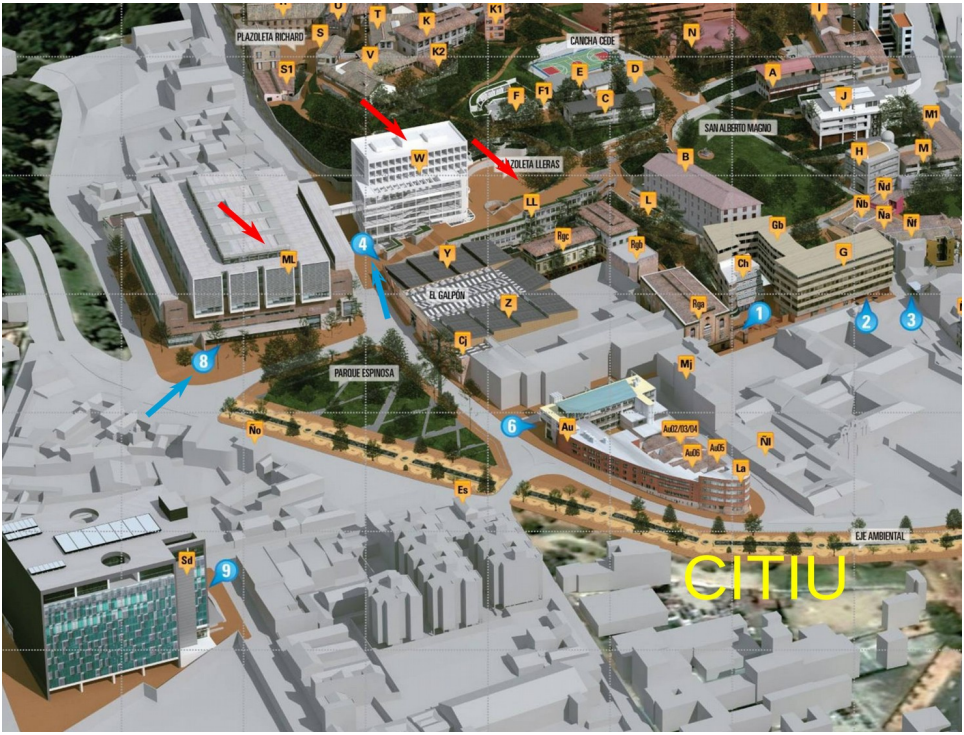
MAPS

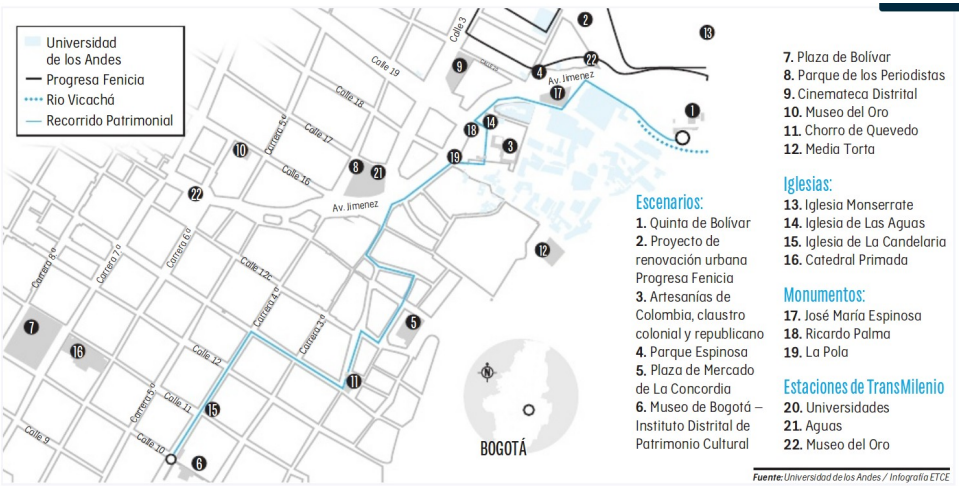
Buildings (red arrows): W, ML, and LL

Entrances (blue arrows):

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

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





Fuente: Universidad de los Andes / Infografía ETCE

PROGRAM 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	Camilo Aponte
			CT: Helman Amaya
15:00 – 15:30	CT: A. Sandoval	CT: Alberto Castillo	José D. Muñoz
15:30 – 16:00	Coffee break	**Poster session**	
16:00 – 17:00	Ulrich Schwarz		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

Monday, September 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		**Camilo Aponte UNIANDES, Bogotá**	*Force-sensitive adhesive blood proteins studied by molecular dynamics simulations*
14:30 – 15:00		**Contributed talk: Helman Sandoval UNIANDES, Bogotá**	*Dynamics of self-interacting bio-inspired polymers in shear flows*
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 Iba-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.*