

# 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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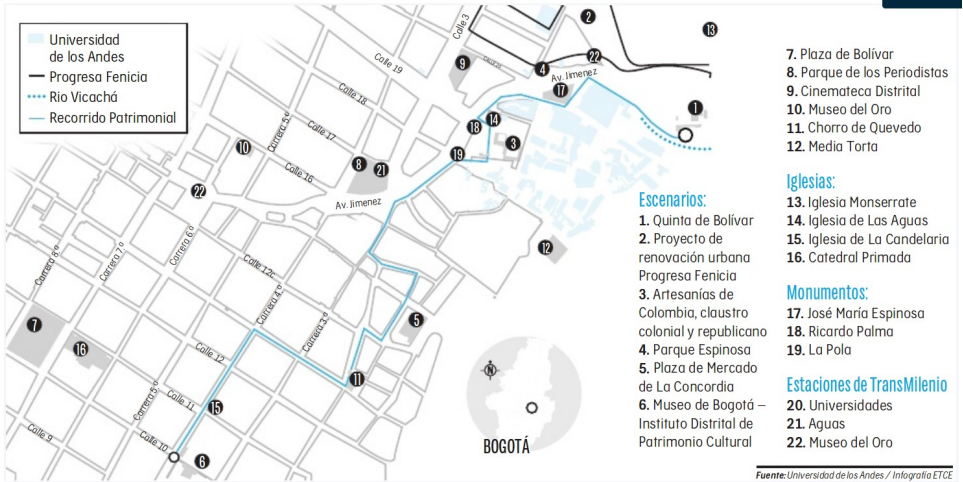
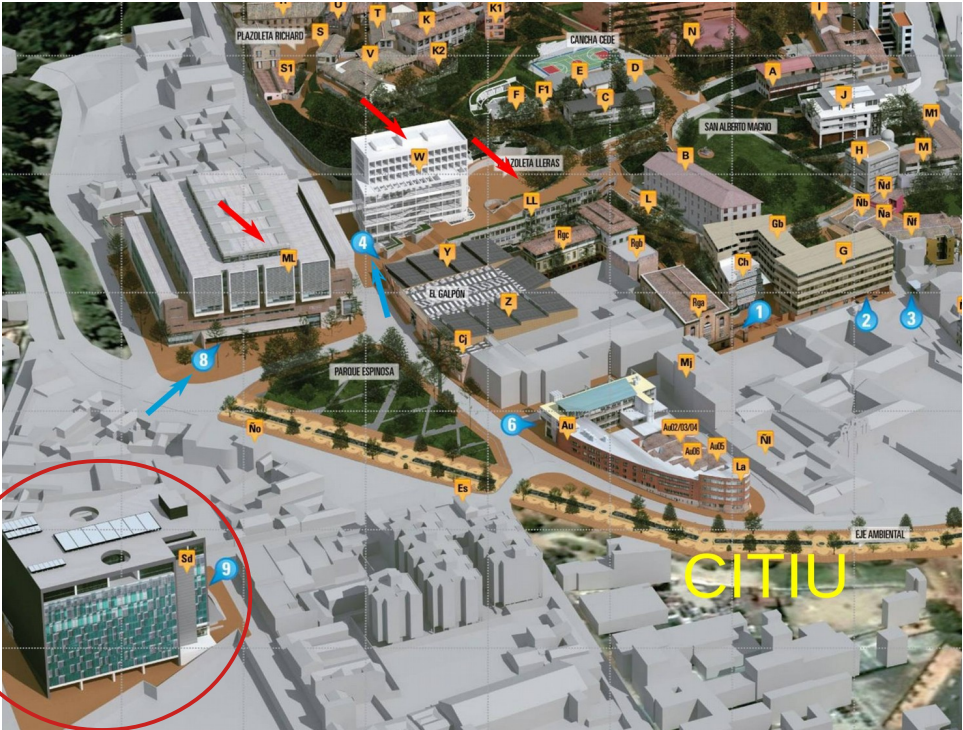
# MISTI



[mptg-cbp.github.io/  
teaching/for-biol-2019](https://mptg-cbp.github.io/teaching/for-biol-2019)



**VENUE:**  
**University of Los Andes, Bogotá, Colombia**  
**SD Building (Cll. 21 # 1-20, Entrance 9 in the map).**  
**Room SD-803**



**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	Ulrich Schwarz	Ulrich Schwarz	CT: Helman Amaya
			CT: Sergio Cruz-León
15:00 – 15:30	CT: A. Sandoval	CT: Alberto Castillo	José D. Muñoz
15:30 – 16:00	Poster session	Coffee break	
16:00 – 17:00		Alfredo Alexander-Katz	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 renowned scientists, 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

8:00 – 9:00	Registration	
9:00 – 9:30	Welcome	
9:30 – 10:30	<b>Helmut Grubmüller MPIBPC, Göttingen</b>	<i>Force-probe molecular dynamics simulations</i>
10:30 – 11:00	Coffee break	
11:00 – 12:00	<b>Frauke Gräter HITS, Heidelberg</b>	<i>Mechanics of focal adhesions and collagen fibers</i>
12:00 – 14:00	Lunch	
14:00 – 15:00	<b>Ulrich Schwarz U. Heidelberg</b>	<i>Introduction to modeling cell mechanics and adhesion</i>
15:00 – 15:30	<b>Contributed talk: Angélica Sandoval. UNIANDES, Bogotá</b>	<i>The interaction of blood proteins with extracellular DNA</i>
15:30 – 15:40	Photo	
15:40 – 17:30	Poster session	
19:00 –	Invited speakers dinner	

### Tuesday, October 1

9:30 – 10:30	<b>Frauke Gräter HITS, Heidelberg</b>	<i>Spider silk and other biomaterials with exceptional mechanical properties</i>
10:30 – 11:00	Coffee break	
11:00 – 12:00	<b>Helmut Grubmüller MPIBPC, Göttingen</b>	<i>Molecular motors &amp; Ribosomal translation</i>
12:00 – 14:00	Lunch	
14:00 – 15:00	<b>Ulrich Schwarz U. Heidelberg</b>	<i>Biophysics of malaria-infected red blood cells</i>
15:00 – 15:30	<b>Contributed talk: Alberto Castillo, UJTL, Bogotá</b>	<i>A parasite's thoughts: What is like to swim inside you?</i>
15:30 – 16:00	Coffee break	
16:00 – 17:00	<b>Alfredo Alexander-Katz. MIT, Cambridge</b>	<i>Adsorption of soft materials under non-equilibrium conditions</i>



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

## POSTERS

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