# Giovanni Di Muccio

#### EDUCATION

Ph.D. in Industrial Engineering, with honors

University of Rome Tor Vergata, Italy

Thesis: Computational Modeling of Nanopore Based-Devices for Protein Sensing and Sequencing.

2017-2021

Ms.C. Nanotechnology Engineering, with honors

Sapienza University of Rome, Italy

Thesis: Acoustically Induced Bjerknes Forces on Encapsulated Gas Microbubbles.

2014-2017

B.Sc. Chemical Engineering,

Sapienza University of Rome, Italy

Thesis: Laminar Flows in Triangular Cross-Section Ducts for Microfluidic Applications.

2009 - 2013

# Research Experience and Main Collaborations

#### University of Rome Tor Vergata

Rome, Italy Postdoctoral Researcher Nov. 2021, May 2022

- Computational analysis of transport mechanism for ions across a cell membrane and role in the cardiovascular system.

University of Rome Tor Vergata

Rome, Italy

Ph.D. Student, advisor Prof. M. Chinappi, co-adv. B. Morozzo della Rocca.

2017-2021

University of Groningen

Remote collaboration, Maglia Lab, Prof. G. Maglia.

Groningen, Netherlands 2021, ongoing

- Computational modeling and Molecular Dynamics simulations of "large" biological nanopores and small globular proteins: structure prediction, capture rates and pore hindrance estimation.
- Electrohydrodynamics characterization of WT and mutated nanopores: electrostatic, ionic selectivity and electroosmotic flow engineering.

#### Université d'Évry/Collège de France

Paris, France Visiting Research, Lambe Lab/Solid State Chemistry and Energy, Profs. J. Pelta and J.M. Tarascon. Winter 2019

- Development of an experimental nanopore sensing setup for electrochemical applications.
- Modeling and characterization of cyclodextrins and polysulfurs molecular interactions.
- Molecular Dynamics simulations of an  $\alpha$ -Hemolysin nanopore at high pH: ionic selectivity and electroosmotic flow estimation.

## Ioan Cuza University

Iasi, Romania

Remote collaboration, Prof. T. Luchian's group.

Summer 2018

- Molecular Dynamics simulations of small dipolar peptides through an  $\alpha$ -Hemolysin nanopore: peptide structure, ionic currents and pore hindrance correlations analysis.

#### CLNS@SAPIENZA, IIT/Sapienza University of Rome

Rome, Italy

Microfluidic Group, Master Thesis, advisor C.M. Casciola, co-adv Prof. M. Chinappi.

Dec-2016, Jul-2017

- Development of an experimental setup of a microfluidic environment mimicking the Blood-Brain Barrier impairmen, for Ultrasounds Microbubbles Targeted Drug-Delivery Studies.
  - \* Eperimental: cultivating and seeding endothelial cells in a microfluidic device.
  - \* Computational: Acoustic propagation modeling of the microfluidic device (COMSOL Multiphysics)
- Acoustofluidic theoretical modeling and experiments of encapsulated-gas microblubbles in confined environment.
  - \* Eperimental: Micro-PIV particle tracking (microbubbles under ultrasounds in confined environment).
  - \* Computational: implementation of modified Reyleigh-Plesset differential equation (radius dynamics of an excited microbubbles) into a particle Euler-Lagrange model, for simulating the collective motion of hundreds of microbubbles (FORTRAN, MATLAB).

# TEACHING AND TUTORING ACTIVITIES

- Tutoring and Orientation Activities at University of Rome Tor Vergata
   Matematica di Base e Orientamento, Undergraduate Level, Macroarea di Ingegneria (POT-ING)

   Supervising Master, PhD and Visiting students,
- teaching Molecular Dynamics simulations, Linux and HPC resources usage and managment.

  Chemical Nano-Engineering & Industrial Engineering at University of Rome Tor Vergata

2020

• Tutor for private lessons

Physics, Chemistry/Biochemistry, Calculus I, Informatic/Coding

2013-Present

# Additional Schools and Trainings

- STIMULATE Workshop: Machine and Reinforcement Learning, Rare Events and Tensor Networks University of Rome Tor Vergata, 2020
- Introduction to Machine Learning, University of Rome Tor Vergata, 2019
- Introduction to modern FORTRAN, CINECA, Bologna, 2018

## TECHNICAL SKILLS

- Scientific Computation: NAMD/VMD, COMSOL Multiphysics, Custom Codes
- Scripting/Programming: Bash, Python, TCL, FORTRAN, R, MATLAB, C/C++, Wolfram Mathematica, Ruby
- Office, Graphics and 3D printing: Microsoft and Open Office, Latex, Inkscape, Blender, ImageJ/Fiji, Gimp

## HPC PROJECTS

• CSGGEOF, MARCONI M100 (Iscra C IsC86), <b>PI</b>	2021
• Geometrically induced selectivity [] in uncharged nanopores, CSCS Piz Daint (s1103), Main Collaborator	2021
• Effect of mutations [] in YaxAB nanopore, CSCS Piz Daint (s1026), Main Collaborator	2020
• FLOWYAX, CINECA M100 (IsB21), Collaborator	2020
• Electroosmotic flow in WT CgsG nanopore, CSCS Piz Daint (s958), Main Collaborator	2019
• Electroosmotic flow in conical nanopores, CSCS Piz Daint (s865), Collaborator	2018

# International Talks

- Transport in Narrow Channels (Invited), Cargse, France, 2022
- ELKIN2022, Tel Aviv, Israel, 2022
- 1st MASBIC-DISVA Symposium, Ancona, Italy, 2021
- FICN2021: Frontiers in ion channels and nanopores, Rome, Italy, 2021
- 2<sup>nd</sup> Single Molecule Protein Sequencing, Jerusalem, Israel, September 2019
- Single Nanopore for Sensing and Energy,
   Université de Montpellier, France, July 2019
- Biophysics@Rome, CNR Headquartes, Rome, Italy, May 2019

## Posters

- Nanopore Sequencing, Boston, USA, 2022
- FICN2021, Rome, Italy, 2021
- 12th EBSA/10th ICPB-IUPAB Biophysics Congress, Madrid, Spain, 2019
- Biophysical Society 63rd Annual Meeting, Baltimore, Maryland, USA, 2019
- Nanoinnovation, Rome, Italy, 2018, 2019, 2020
- Nanofluidic in Physics and Biology, Lyon, France, 2018

### LANGUAGES

• Italian: Mother tongue

• English: Proficient in both written and spoken language

### AWARDS AND HONORS

• FICN2021, Rome, Italy, 2021 Best Poster Award

# **PUBLICATIONS**

- [1] Geometrically Induced Selectivity and Unidirectional Electroosmosis in Uncharged Nanopores.
- G. Di Muccio, B. Morozzo della Rocca, Acs Nano, 2022
- [2] Electroosmosis in nanopores: Computational methods and technological applications
- A. Gubbiotti, M. Baldelli, G. Di Muccio, P. Malgaretti, S. Marbach, M. Chinappi, Advances in Physics: X, 2022
- [3] Nanopore-based protein sequencing using biopores: current achievements and open challenges.
- A. Asandei, G. Di Muccio, I. Schiopu, L. Mereuta, I. S. Dragomir, M. Chinappi, SMALL METHODS, 2020
- [4] Single-sulfur atom detection of polysulfides with a protein nanopore for improved batteries.
- F. Btermier, B. Cressiot, G. Di Muccio et al., NATURE COMMUNICATION MATERIALS, 2020
- [5] Insights into protein sequencing with an -Hemolysin nanopore by atomistic simulations.
- G. Di Muccio, A.E. Rossini, D. Di Marino, G. Zollo, M. Chinappi, Scientific Reports, 2019
- [6] Single-molecule dynamics and discrimination between hydrophilic and hydrophobic amino acids in peptides, through controllable, stepwise translocation across nanopores.
- A. Asandei, I.S. Dragomir, G. Di Muccio et al., Polymers, 2018