Raúl Pérez Peláez

*I am interested in the **modeling and simulation of biologically-relevant soft matter systems**. I build integrated machine-experiment models and **high-performance software** tools that quantitatively predict properties of complex fluids for biomedical applications. I navigate the intersection between physics, applied-math, computer science and biology.*

Location: Madrid, Spain
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Google Scholar: Raul P. Pelaez

Academic Background

2010 – 2014 **Physics degree**
Universidad Autonoma de Madrid

2015 – 2016 **Master in Physics of Condensed Matter and Biological Systems**
Universidad Autonoma de Madrid

2018 – 2022 **Ph.D. in Physics (High Performance simulation of Soft Matter and Complex Systems)**
Universidad Autonoma de Madrid. Director: Prof. Rafael Delgado-Buscalioni

Ph.D. Thesis

Title	Complex fluids in the GPU era: Algorithms and simulations
Supervisor	Professor Rafael Delgado-Buscalioni
Short description	Developed advanced mathematical and algorithmic frameworks for simulating complex fluid systems in Graphical Processor Units, focusing on two-phase interactions (solid-liquid) governed by thermal fluctuations and hydrodynamic correlations (such as many biological systems). My contributions include UAMMD, a high-performance CUDA-based simulation engine designed for efficient modeling of complex fluids, setting new standards in computational soft matter physics.

Communication skills

English	Fluent
Spanish	Mother tongue

Selected software skills

Guru	C++20, CUDA, Python, PyTorch, UNIX, emacs, CMake, git
Advanced	Regex, SYCL, Latex, OpenMP, OpenGL 3.3+, C, Matlab
Intermediate	Perl, MPI, GLSL, Java, SDL2, inkscape, gimp, Arduino, gdb, SFML, OpenCL, JAX, Javascript
Basic	Android, Fortran, PowerShell, Triton

I am able to properly apply hygienic software engineering principles to software projects of any size from the ground up.

Areas of Interest

- High performance scientific computing and GPU programming.
- Complex fluids and fluctuating hydrodynamics.
- Modeling and simulation of biological systems.
- Machine learning.

- Software engineering.

Research experience

October 2014 – May 2015

Lab technician

Obtaining graphene samples by mechanical exfoliation for high speed AFM studies. Hired by Dr. Julio Gómez in Universidad Autónoma de Madrid.

May 2015 – 2017

Software technician

Developing high performance GPU software for molecular dynamics in the Condensed Matter Theoretical Physics department at the Universidad Autonoma de Madrid. Focusing in the areas of complex fluids and colloids. Developing for both simulation and visualization of data.

2018 – 2021

Ph.D. student

Working towards a Ph.D. in the Condensed Matter Physics, Nanoscience and biophysics program at Universidad Autonoma de Madrid. Under the supervision of Professor Rafael Delgado-Buscalioni. In the area of Complex fluids and colloidal systems, developing new algorithms for fluid-matter interaction using Graphical Processor Units.

2021 – 2022

Postdoctoral research assistant

Working with Prof. Aleksandar Donev at the Courant institute (New York University) as a research assistant specialized in GPU HPC software for fluctuating hydrodynamics.

2022 – 2023

Postdoctoral researcher

Developing high performance GPU software for biosensor simulation with Prof. Rafael Delgado-Buscalioni at the Universidad Autonoma de Madrid.

2023 – 2024

Research director

Developing high performance GPU software at Universitat Pompeu Fabra with Prof. Gianni de Fabritiis. The role focused on Machine Learning software for drug discovery tasks and biomolecular simulations, including the development of the neural network potential capabilities of the OpenMM toolkit.

2024 – present

Adjunt professor

Lecturing at the IE School of Science and Technology. Teaching courses on programming and physics labs.

Contribution to Open Source software projects

I have written and contributed to many open-sourced scientific software. The majority of it is available at my Github profile (`github.com/RaulPPelaez`). Here, I showcase some of my most beloved projects:

github.com/RaulPPelaez/UAMMD

UAMMD - Universally Adaptable Multiscale Molecular Dynamics

I developed this project as a part of my Ph.D. UAMMD is a CUDA/C++ library for complex fluid simulation, focused on fluctuating hydrodynamics. UAMMD plays a fundamental role in several research groups around the globe.

GITHUB.COM/TORCHMD/TORCHMD-NET

TorchMD-NET

TorchMD-NET provides state-of-the-art neural networks potentials (NNPs) and a mechanism to train them. It offers efficient and fast implementations if several NNPs and it is integrated in GPU-accelerated molecular dynamics code like ACEMD, OpenMM and TorchMD. TorchMD-NET exposes its NNPs as PyTorch modules.

GITHUB.COM/OPENMM/OPENMM

OpenMM

OpenMM is a popular high performance toolkit for molecular simulation. I acted as a research director for the OpenMM project during my time at the Universitat Pompeu Fabra (UPF), where I held a key role in the development of the OpenMM machine learning stack, among other things.

GITHUB.COM/RAULPPELAEZ/SUPERPUNTO

Superpunto - A particle visualizator

I developed this project during my Masters, and while it is testament to my lack of experience at the moment I hold it very dearly. Superpunto is a particle visualizator written in C++ using OpenGL 4.5. It allows for fast visualization of simulation results in the form of spherical particles.

COMMUNICATION

SELECTED CONTRIBUTIONS TO INTERNATIONAL CONFERENCES AND WORKSHOPS

- **Soft Matter and Nanofluids at the Multiscale** - Workshop - Madrid (2015). *Poster presentation.*
- **FISES18** - Statistical physics conference - Madrid (2018). *Poster presentation.*
- **Jornada INC 2018** - Physics - Madrid (2018). *Poster presentation.*
- **Biological and bio-inspired materials: from responsiveness to activity. EBSA, IUPAP** - Biophysics workshop - Madrid (2019). *Oral presentation.*
- **12th EBSA 10th ICBP-IUPAP Congress** - Biophysics conference - Madrid (2019). *Poster presentation.*
- **Nanomaterials Applied to Life Sciences 2020 (NALS2020)** - Nanomaterials conference - Madrid (2020). *Oral presentation.*
- **VI Workshop de la Red de Simulación Molecular** - Molecular simulation workshop - Baiona, Spain (2021). *Oral presentation.*
- **From Stokesian suspension dynamics to particulate Flows in turbulence** - Conference - Toulouse, France (2022). *Oral presentation.*
- **FISES22** - Statistical physics conference - Madrid, Spain (2022). *Poster presentation.*
- **SFMC22** - Fluid mechanics conference - Cadiz, Spain (2022). *Poster presentation (best poster award).*
- **Methods in Molecular Simulations And Machine Learning** - Conference - Barcelona, Spain (2022). *Poster presentation.*
- **Computational methods and tools for complex suspensions** - Workshop - Bilbao. Spain (2022). *Software tutorial and poster.*
- **SYCLCON 2023** - HPC Conference - Cambridge, UK (2023). *Attendant*
- **First Dynamics of Non-Equilibrium Variables (DoNEV) meeting** - Conference - Zaragoza, Spain (2025). *Organizer.*

INVITED TALKS AND VISITS

- GPU accelerated simulations of complex fluids - Imperial College - London, UK (2023).
- Machine learning potentials for molecular dynamics - MINES - Colorado, USA (2024).
- Practical software engineering for software-writing scientists - MINES - Colorado, USA (2024).

List of selected publications

Number of citations up until June 18, 2025 between parenthesis in bold.

(58) OpenMM 8: molecular dynamics simulation with machine learning potentials
P. Eastman, R. Galvelis, R. P. Peláez, C. R. A. Abreu, S. E. Farr, E. Gallicchio, A. Gorenko, M. M. Henry, F. Hu, J. Huang, ...
The Journal of Physical Chemistry B, 128 (1), 109–116, 2023

(19) A fast spectral method for electrostatics in doubly periodic slit channels
O. Maxian, R. P. Peláez, L. Greengard, A. Donev
The Journal of Chemical Physics, 154 (20), 2021

(15) Simulations of dynamically cross-linked actin networks: morphology, rheology, and hydrodynamic interactions
O. Maxian, R. P. Peláez, A. Mogilner, A. Donev
PLoS Computational Biology, 17 (12), e1009240, 2021

(15) Upconverting nanorockers for intracellular viscosity measurements during chemotherapy
P. Rodríguez-Sevilla, F. Sanz-Rodríguez, R. P. Peláez, R. Delgado-Buscalioni, L. Liang, X. Liu, D. Jaque
Advanced Biosystems, 3 (10), 1900082, 2019

(13) TorchMD-Net 2.0: Fast Neural Network Potentials for Molecular Simulations
R. P. Peláez, G. Simeon, R. Galvelis, A. Mirarchi, P. Eastman, S. Doerr, P. Thölke, T. E. Markland, G. De Fabritiis
Journal of Chemical Theory and Computation, 2024

(12) Hydrodynamic fluctuations in quasi-two dimensional diffusion
R. P. Peláez, F. B. Usabiaga, S. Panzuela, Q. Xiao, R. Delgado-Buscalioni, A. Donev
Journal of Statistical Mechanics: Theory and Experiment, 2018 (6), 063207, 2018

(10) Collective colloid diffusion under soft two-dimensional confinement
S. Panzuela, R. P. Peláez, R. Delgado-Buscalioni
Physical Review E, 95 (1), 012602, 2017

(8) Optofluidic control of the dispersion of nanoscale dumbbells
M. Meléndez, N. Alcázar-Cano, R. P. Peláez, J. J. Sáenz, R. Delgado-Buscalioni
Physical Review E, 99 (2), 022603, 2019

(7) Computing hydrodynamic interactions in confined doubly periodic geometries in linear time
A. Hashemi, R. P. Peláez, S. Natesh, B. Sprinkle, O. Maxian, Z. Gan, A. Donev
The Journal of Chemical Physics, 158 (15), 2023

(5) Complex fluids in the GPU era: Algorithms and simulations
R. P. Peláez
Universidad Autónoma de Madrid, 2022

(4) Predicting the size and morphology of nanoparticle clusters driven by biomolecular recognition
P. Palacios-Alonso, E. Sanz-de-Diego, R. P. Peláez, A. L. Cortajarena, F. J. Teran, R. Delgado-Buscalioni
Soft Matter, 19 (46), 8929–8944, 2023

(3) Origin of tank-treading and breathing dynamics of star polymers in shear flow
R. P. Peláez, R. Delgado-Buscalioni
Macromolecules, 53 (7), 2634–2648, 2020

(1) Universally Adaptable Multiscale Molecular Dynamics (UAMMD): A native-GPU software ecosystem for complex fluids, soft matter, and beyond
R. P. Peláez, P. Ibáñez-Freire, P. Palacios-Alonso, A. Donev, R. Delgado-Buscalioni
Computer Physics Communications, 306, 109363, 2025

(1) On the Inclusion of Charge and Spin States in Cartesian Tensor Neural Network Potentials
G. Simeon, A. Mirarchi, R. P. Peláez, R. Galvelis, G. De Fabritiis
arXiv preprint, arXiv:2403.15073, 2024