

Raúl Pérez Peláez

I am interested in the **modeling and simulation of biologically-relevant systems**. I build integrated machine-experiment models and **high-performance software** tools that adhere to healthy software engineering practices and quantitatively predict properties biomedical systems. I navigate the intersection between physics, applied-math, computer science and biology.

🏠 Location: Madrid, Spain
🌐 <https://github.com/RaulPPelaez>
✉ contact@raulppelaez.com
🎓 Google Scholar: Raul P. Pelaez

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, WebAssembly, WebGPU, WebGL, Numba
INTERMEDIATE Perl, MPI, Java, SDL2, inkscape, gimp, Arduino, gdb, SFML, OpenCL, JAX, Javascript/Typescript
BASIC Android, Fortran, PowerShell, Triton, WebUSB, TinyGrad, React

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

DevOps tools: GitOps, CI/CD (GitHub Actions), Docker/Compose, pip, conda, npm, SLURM, Ansible.

AREAS OF INTEREST

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

WORK EXPERIENCE

High Performace Software Engineer

2026 – PRESENT



• Developing WebGPU code for High Performance 3D graphics

Adjunt professor

2024 – PRESENT



Lecturer (Adjunct) in the Computer Science and Applied Math degrees. Teaching courses such as:

- Computer Programming 2 (compsci): C++
- Computer Programming 2 (applied math): Advanced Python
- Computer Programming 1 (compsci): Advanced C

Research scientist



- Developed several GPU-ready open source tools for high-performance scientific computing (C++/CUDA with Python wrappers).
- Set up CI/CD GitHub actions with custom runners for automatic testing and benchmarking in a local GPU cluster (100 GPUs).
- Developed new massively parallel algorithms for biosensor modelling, published in scientific journals.
- Wrote a high-performance web application (WebAssembly via C++ with Emscripten, WebGPU, Astro/React) for a digital twin product.
- Developed and implemented high-performance algorithms for research in liquid memory storage.
- Mentored several PhD students.

2023 – 2024

Research director

Provide core GPU libraries and tooling to research groups, industry, and OSS projects, mainly for AI-assisted molecular modeling and drug-discovery.

Actions

- Implemented custom torch.compile-ready, Autograd-enabled, CUDA ops in TorchMD-Net; profiled and refactored neighbor search path with nsight compute.
- Wrote and maintained conda-forge recipes for OpenMM, TorchMD-Net, OpenMM-Torch, CUTLASS, pyg-lib, NNPOPS, and more.
- Integrated CUDA Graphs into OpenMM-Torch for smoother ML-augmented MD runs.
- Built CI/CD matrices (GitHub Actions) with GPU, CPU, and cross-platform wheels, plus auto-generated docs.
- Ported Neural Network Potential ML models to JAX, TinyGrad, and TensorFlow.
- Wrote a Slack App integrating a local LLM model acting as an assistant in the internal workspace. The backend LLM model offered functionality such as tool usage, RAG, model hot-swap, paper summarization, and more. The LLM ran in an in-house GPU computing cluster, capable of hosting sub-60b parameter models (Llama family, Mistral,...).
- Finetuned LLM models for custom workflows in drug discovery.

Impact

- TorchMD-Net inference time reduced from hours to minutes (50 x speed-up).
- conda-forge packages adopted by multiple bio-physics labs; eased deployment on HPC clusters.



2022 – 2023

Postdoctoral researcher



Research software engineer and postdoctoral researcher. Also took care of the local GPU computing cluster.

- Managed a SLURM HPC cluster with 600 CPU cores and 40 NVIDIA GPUs scattered around 15 computing nodes.

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.

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.

MAY 2015 – 2017

Software technician

SELECTED 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](https://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](https://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 of 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](https://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](https://github.com/RaulPPelaez/Superpunto)

Superpunto - A particle visualizer

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 visualizer written in C++ using OpenGL 4.5. It allows for fast visualization of simulation results in the form of spherical particles.

ACADEMIC BACKGROUND

- 2010 – 2014 **Physics degree**
Universidad Autónoma de Madrid
- 2015 – 2016 **Master in Physics of Condensed Matter and Biological Systems**
Universidad Autónoma de Madrid
- 2018 – 2022 **Ph.D. in Physics (High Performance simulation of Soft Matter and Complex Systems)**
Universidad Autónoma 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

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 March 16, 2026 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