Curirriculum Vitae Gianmarco Accordi

1 Contacts

Email	gianmarco.accordi@polimi.it
Phone	+39 349 5375363
Linkedin	gianmarco-accordi
Website	www.gianmarcoaccordi.info
GitHub	gianfi12

2 Short Bio

I've completed my Master's and Bachelor's degree at Politecnico di Milano, with a thesis titled "*A High-throughput pose selection method for extreme scale virtual screening in drug discovery*". Currently, I am a PhD student at Politecnico di Milano, and my research thesis is about the acceleration and performance portability of virtual screening applications on emerging HPC architectures. Specifically, I am part of the development team of LiGen, a high-throughput, extreme-scale virtual screening pipeline. LiGen has been used in the largest virtual screening campaign against SARS-CoV-2, the context of the European project EXSCALATE4CoV. In particular, I focus on the porting and optimization of computation kernels on GPUs. My research interests also include the integration of AI modules into virtual screening applications and the analysis of their accuracy and performance.

3 Working Experience

Research Fellow
at Politecnico di Milano *2022 - Present*
I'm responsible for designing, implementing, and evaluating techniques to optimize virtual screening applications on modern EuroHPC supercomputers.

Teaching Assistant
at Politecnico di Milano *2022 - Present*
I've been a lecturer in various computer science courses on C, Python, and GPU programming.

Full Stack Engineer Specialist
at Mia-Platform *2022*
I've worked as a DevOps, focusing on maintaining and developing the ticket-selling system for a railway company. My main contribution has been designing and implementing a comprehensive digital selling system for passes.

Internship
at MobiMESH *2017*
The intern's objective was to analyze and design tools and software for a Wireless captive portal for many clients.

4 Education

PhD's student in Computer Science and Engineering
Politecnico di Milano *2022 - Present*

Master's degree in Computer Science and Engineering
Politecnico di Milano *2019 - 2022*

Bachelor's degree in Computer Science and Engineering
Politecnico di Milano *2016 - 2019*

5 Skills

OS	Linux, Windows, MacOS
Languages	C/C++, Python, Fortran, Bash
Parallel Programming	CUDA, OpenMP, OpenACC, OpenCL, HIP, MPI, SYCL
Compiler	NVCC, Clang, GCC, LLVM
AI	PyTorch, TensorFlow, Numpy, Pandas, DGL
Cheminformatics	LiGen, AutoDock, PyMOL
Project Management	Git, Jira
ISA	x86, PTX, ARM
Job Scheduler	SLURM, PBS

6 Selected Papers

1. *GPU-optimized Approaches to Molecular Docking-based Virtual Screening in Drug Discovery: A Comparative Analysis*
   Submitted to Journal of Parallel and Distributed Computing, 2023

2. *Out of Kernel Tuning and Optimizations for Portable Large Scale Docking Experiments on GPUs*
   Submitted to The Journal of Supercomputing, 2023

3. *Enabling Performance Portability on the LiGen Drug Discovery Pipeline*
   Submitted to Future Generation of Computer Systems, 2023

4. *Domain-Specific Energy Modeling for Drug Discovery and Magnetohydrodynamics Applications*
   Supercomputing, 2023