

Curriculum Vitæ et Studiorum



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Short Bio

Davide Gadioli received his Ph.D. cum laude in Information Technology from Politecnico di Milano in 2019. His early research focused on dynamic application autotuning, with particular emphasis on performance–quality trade-offs, including a real-world virtual screening use case. He later specialized in high-performance computing (HPC) application optimization and high-throughput virtual screening for extreme-scale drug discovery. Since 2018, he has been part of the team leading the development of the structure-based virtual screening software for the EXaScale smArt pLatform Against paThogEns (EXSCALATE). In 2021, he contributed to the largest virtual screening experiment conducted against 15 targets across 12 SARS-CoV-2 viral proteins. Currently he is a junior assistant professor at Politecnico di Milano.

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Position and Education

RECORD OF EMPLOYMENT

06/2024 – present

Junior Assistant Professor at the Department of Electronics, Information and Bioengineering (DEIB) of the Politecnico di Milano.

The carried-out activities include the optimization of a extreme-scale virtual screening campaign in the context of urgent computing.

05/2021 – 05/2024

Postdoctoral Researcher in Computer Engineering at the Department of Electronics, Information and Bioengineering (DEIB) of the Politecnico di Milano working on “Sviluppo di una piattaforma di drug-discovery per sistemi ad alte prestazioni per il progetto LIGATE. Ottimizzazione dei moduli software usando tecniche di tuning automatico e intelligenza artificiale”

The carried-out activities include re-designing computing methodologies for the extreme-scale scenario in High-Performance Computing systems, to improve the “EXaScale smArt pLatform Against paThogEns” (EXSCALATE), in the context of the “Ligand Generator and portable drug discovery platform AT Exascale” (LIGATE) European Project.

11/2017 – 04/2021

Postdoctoral Researcher in Computer Engineering at the Department of Electronics, Information and Bioengineering (DEIB) of the Politecnico di Milano working on “Ottimizzazione automatica delle applicazioni nell’ambito di sistemi dedicati e ad elevate prestazioni”

The carried-out activities include proposing, analyzing, developing, and evaluating techniques to optimize and improve the EXSCALATE platform, in the context of the ANTAREX and LIGATE European Projects. Contribute to the largest virtual screening simulation against 12 viral proteins of SARS-CoV-2, in the context of the “EXSCALATE4CoV” European Project.

09/2015 – 11/2015

Internship at IBM Research, Amsterdam, The Netherlands, working on the analysis of application-specific optimizations at the code level and their effects concerning the scaling of multi-threaded applications towards exascale computing.

01/2014 – 11/2014

Fellow Researcher in Computer Engineering at the Department of Electronics, Information and Bioengineering (DEIB) of the Politecnico di Milano working on “Monitoraggio delle proprietà extra-funzionali in sistemi multiprocessore con capacità di adattamento.”

The carried-out activities include developing an extra-functional property monitoring layer on top of an ultra-low-power sensor node, in the context of the European Project “Design of embedded mixed-criticality CONTROL systems under consideration of EXtra-functional properties” (CONTREX)

EDUCATION

- Ph.D. *cum laude* in Information Technology at Politecnico di Milano in 2019.
Thesis Title: *Dynamic application autotuning for self-aware approximate computing*
Advisor: Prof. Gianluca Palermo
Award: Springer Award - Ph.D. thesis published in Polimi SpringerBriefs

- Master of Science degree in Information Technology in 2013
Thesis title: *ARGO: un framework per il supporto all'adattabilità di applicazioni in architetture multi-processore*,
Advisor: Prof. Gianluca Palermo

Awards

- AW.1. HiPEAC Technology Transfer Award 2020 for the technology - "GeoDock: A Fast and Configurable Pocket-Aware Ligand Pose Generator for High-Throughput Molecular Docking".
- AW.2. EU Innovation Radar - mARGOt autotuning framework has been analysed by the European Commission's Innovation Radar and categorized as "Tech Ready" and with a "Very High" innovation potential.
- AW.3. Springer Award - Published the results of the Ph.D. thesis in the Polimi SpringerBriefs volume.

Professional Activities

TECHNOLOGY TRANSFER

- GeoDock - Fast and Configurable Pocket-Aware Ligand Pose Generator for High-Throughput Molecular Docking - Technology transferred to DOMPE' Farmaceutici (HiPEAC Technology Transfer Award 2020) - Type: Software
- libdpipe - A library that provides the facilities required to implement an application that can scale up and out to exploit an HPC supercomputer - Technology transferred to DOMPE' Farmaceutici - Type: Software
- LiGen-HT - High-Throughput implementation of the LIGEN platform for the virtual screening that can scale up to an entire supercomputing center - Technology transferred to DOMPE' Farmaceutici - Type: Software
- LiGen-Pocket - A library that pre-computes protein's properties to enable High-Performance virtual screening campaigns - Technology transferred to DOMPE' Farmaceutici - Type: Software
- Adaptive PTDR - Automatically tune a probabilistic time-dependent routing application using input features to increase computation efficiency - Technology transferred to IT4Innovations - Type: Software
- mARGOt - Adaptation layer that enhances an application with the self-optimization capability - Open source repository: https://gitlab.com/margot_project/core (EU Innovation Radar) - Type: Software
- GPU-Accelerated 3D Hologram Library - the technology has been transferred to ESSILOR-LUXOTTICA within the context of the industrial project "Code Porting and Optimization on Parallel Architectures (e.g. GPUs) for a 3D Hologram Application"

SERVICES IN JOURNALS AND CONFERENCES

Workshop organizer

- The first workshop on Scalable Performance, Portability, and Productivity for Scientific Computing SP4Sci '26. Co-located with Computing Frontiers.

Guest Editor

- Special Issue named “Advances in Scientific Applications toward High-Performance Computing” in the journal Electronics - MDPI

Conferences and Workshops as external reviewer or sub-reviewer (not in the TPC)

- SpringerOpen Journal of Big Data; Elsevier Microprocessors and Microsystems; HiPC (2021, 2022) - IEEE International Conference on High-Performance Computing, Data, and Analytics; CODES+ISSS (2017–2021) - International Conference on Hardware/Software Codesign and System Synthesis; FPL (2019 – 2020) - International Conference on Field-Programmable Logic and Applications; DATE (2017 – 2020) - Design Automation and Test in Europe; IC-SAMOS (2019 – 2021) - International Conference on Embedded Computer Systems: Architectures, Modeling and Simulation

National and International Research Projects

SCIENTIFIC RESPONSIBILITY AND PARTICIPATION TO INTERNATIONAL RESEARCH PROJECTS

- *H2020-JTI-EuroHPC-956137-LIGATE - “Ligand Generator and portable drug discovery platform AT Exascale”* - Period: 2021-2023

Role: Task leader

Activities: LIGATE project extends the EXSCALATE platform with the primary objective to exploit the potential of supercomputing combined with life science scientific skills in Europe to better and quickly face pandemic situations of supranational interest. In particular, the coordinated PoliMi activities are the following: (i) the optimization and tuning of parallel applications, and in particular the EXSCALATE platform, on novel heterogeneous architectures; (ii) the development of the molecular docking procedure with the integration of Machine Learning techniques always keeping in mind the urgent computing scenario.

- *H2020-SCI-PHE-CORONAVIRUS-101003551-EXSCALATE4CoV - “EXaScale smArt pLatform Against paThogEns for Corona Virus”* - Period: 2020-2021

Role: Task leader

Activities: The goal of the project is the usage of supercomputers to support the development of novel therapeutic solutions to Covid-19. In particular, the coordinated activity is composed of the porting and continuous optimization of the exascale virtual screening software within the EXSCALATE platform, targeting different European supercomputers and considering the urgent scenario.

- *H2020-FETHPC-671623-ANTAREX - “AutoTuning and Adaptivity appRoach for Energy efficient eXascale HPC systems”* (FET Project) - Period: 2015-2019

Role: Task Leader

Activities: Development of a self-adaptive application-level framework for energy efficient execution in

HPC platforms. The framework exploits autonomous and approximate computing concepts by tuning application-level knobs according to dynamically changing functional and extra-functional requirements.

- *FP7-ICT-611146-CONTREX - “Design of embedded mixed-criticality CONTROL systems under consideration of EXtra-functional properties” (IP Project) - Period: 2013-2016*
Role: Team member
Activities: Design and implementation of an application-level run-time monitoring framework for the extra-functional properties

RESOURCE ALLOCATION PROJECTS SUBJECT TO PEER-REVIEW

- *EHPC-BEN-2022B12-001 (EuroHPC Benchmark Access): “Benchmarking a portable drug discovery platform for Urgent computing” - Period: 03.2023-06.2023*
Role: Co-PI
Resources: 1.280.000 core hours on the LUMI-G partition
Activities: This project aims to benchmark the EXSCALATE virtual screening application on the GPU partition of the LUMI supercomputer, which uses AMD cards. For this reason, the goal was to test and benchmark the SYCL implementation of the computation kernels developed in the context of the LIGATE project.
- *EHPC-DEV-2021D02-049 (EuroHPC Development Access): “Automated Workflow for Computer Accelerated Drug Discovery on Exascale Machines” - Period: 02.2022-02.2023*
Role: Team member
Resources: 1.920.000 CPU core hours, 384.000 GPU core hours
Activities: This project aims to automate the drug design process by minimizing the human effort required in the different phases of the process, including input parameters preparation, the management of data sets with billions of molecules, and the interaction with queue managers to handle jobs.

INDUSTRY-FUNDED RESEARCH PROJECTS

- *High Performance Virtual Screening Software Development and Optimization in the context of the EXSCALATE platform (DOMPE’ Farmaceutici) - 2026*
Role: Co-PI
Activities: The objective is to continue to support DOMPE’ farmaceutici to consolidate the existing EXSCALATE platform to become production ready and to start to design and optimize new domain functionalities to make them HPC ready.
Funding: 210.000€
- *Code Porting and Optimization on Parallel Architectures (e.g. GPUs) for a 3D Hologram Application (EssilorLuxottica) - Period: March-October 2024*
Role: Co-PI
Activities: The objective of this project is to assist EssilorLuxottica in accelerating an application that computes 3D holograms using three distinct algorithms. The target platforms are lower-end GPUs and consumer-grade CPUs. The activity involve porting and optimizing the algorithms using C++ and CUDA.
Funding: 38.500€
- *High-Performance Virtual Screening Software Development and Optimization in the context of the EXSCALATE platform (DOMPE’ Farmaceutici) - Period: 2023-2025*
Role: Task leader
Activities: This project wants to continue the fruitful collaboration between PoliMi and DOMPE’ farmaceutici around the LiGen software as part of the EXSCALATE (EXaScale smArt pLatform Against

paThogEns - www.exscalate.eu) platform. The activities are related to the design of a virtual screening software for drug discovery making efficient use of the underlying computing architectures. The use of the different HPC platforms available in Europe by improving the portability of the code together with its tuning and acceleration are key concepts within the project.

- *High-Performance Virtual Screening Software Optimization for Urgent Computing (DOMPE' Farmaceutici)* - Period: 2020-2022

Role: Task leader

Activities: Design and optimization of a novel geometric docking application for drug discovery in the context of the EXSCALATE (EXaScale smArt pLatform Against paThogEns - www.exscalate.eu) framework. The activity includes the porting of the software in novel HPC node architectures using GPUs. Autotuning techniques and approximate computing approaches will be adopted and studied for speeding up the computation in the context of Urgent Computing.

Talks and Tutorials

INVITED TALKS

- “A Portable Drug Discover Platform for Urgent Computing” at the *EuroHPC User Day*, Bruxelles - Belgium, 2023
- “Autotuning and adaptivity in energy-efficient exascale HPC systems” at the *HPCAFE-2017: High-Performance Computing Approaches for Monitoring, Exploring, Optimizing and Autotuning* (European HPC Summit Week), Barcellona - Spain, 2017

TUTORIALS

- “Runtime Autotuning: the mArgot approach” at the *PRACE On Demand Training Event/School on Monitoring, Compilation and Autotuning Approach for Energy-Efficient HPC Systems*, Ostrava - Czech Republic, 2018
- “Runtime Autotuning: the mArgot approach” within the “The ANTAREX Approach to Adaptively Optimize and Enforce Extra-Functional Properties on HPC Applications” tutorial at the *International Conference on Parallel Architectures and Compilation Techniques - PACT18*, Limassol - Cyprus, 2018.

Teaching Activities

TEACHING PRIMARY RESPONSIBILITY

- Informatica B
Politecnico di Milano - Energy and Mechanical Engineering - Undergraduate level
Academic Year: 25/26

TEACHING ASSISTANT/TUTOR

- Advanced Algorithms and Parallel Programming
Politecnico di Milano - Computer Science and Engineering - Graduate level
Politecnico di Milano - Music and Acoustic Engineering - Graduate level
Course Responsible: Prof. Fabrizio Ferrandi
Academic Year: 23/24, 24/25, 25/26
- Algorithm and Parallel Computing
Politecnico di Milano - Mathematical Engineering- Graduate level
Course Responsible: Prof. Matteo Rossi
Academic Year: 24/25
- Architettura dei Calcolatori e Sistemi Operativi
Politecnico di Milano - Computer Science and Engineering - Undergraduate level
Course Responsible: Prof. Cristina Silvano
Academic Year: 14/15, 15/16, 16/17, 17/18, 18/19, 19/20, 20/21, 21/22
- Informatica B - Informatica per Applicazioni Scientifiche e Industriali
Politecnico di Milano - Engineering Physics - Graduate level
Course Responsible: Prof. Gianluca Palermo
Academic Year: 14/15
- Computing Systems for Engineering Physics
Politecnico di Milano - Engineering Physics - Graduate level
Course Responsible: Prof. Gianluca Palermo
Academic Year: 15/16 16/17 17/18 18/19
- Coding
Politecnico di Milano - TechCamp - High-school level
Course Responsible: Prof. Gianluca Palermo
Period: Summer 2019

STUDENT SUPERVISION

PhD Students Supervision

- *Gianmarco Accordi - Co-Advisor, 2022 – present*
Title: “Approximate Computing in HPC-based Drug Discovery”

Graduate Students Supervision

- He co-advised 9 students at Politecnico di Milano.

Publication List

International journals _____ (# 19)
International book chapters _____ (# 1)
International conferences and workshops _____ (# 21)

REFEREED INTERNATIONAL JOURNALS

- JR.1. Domenico Bonanni, Yuedong Zhang, Davide Gadioli, Gianluca Scarpellini, Pietro Morerio, Alessio Del Bue, Andrea Rosario Beccari, Gianluca Palermo “Condensation of Force Field Parameters from Machine Learning Predicted Distributions for High-Throughput Virtual Screening Applications“. *Journal of Chemical Information and Modeling*, Vol 65/Issue 23, 21 November 2025.
DOI: <https://doi.org/10.1021/acs.jcim.5c02199>
- JR.2. Giovanni Bocchi, Patrizio Frosini, Alessandra Micheletti, Alessandro Pedretti, Gianluca Palermo, Davide Gadioli, Carmen Gratteri, Filippo Lunghini, Akash Deep Biswas, Pieter F. W. Stouten, Andrea R. Beccari, Anna Fava, Carmine Talarico “GENEOnet: a breakthrough in protein binding pocket detection using group equivariant non-expansive operators“. *Nature Scientific Reports*, Sci Rep 15, 03 October 2025.
DOI: <https://doi.org/10.1038/s41598-025-18132-5>
- JR.3. Yuedong Zhang, Gianmarco Accordi, Davide Gadioli, Gianluca Palermo “Harnessing quality-throughput trade-off in scoring functions for extreme-scale virtual screening campaigns“. *Future Generation Computer Systems*, Vol. 172, 28 April 2025.
DOI: <https://doi.org/10.1016/j.future.2025.107863>
- JR.4. Bruno Guindani, Davide Gadioli, Roberto Rocco, Danilo Ardagna, Gianluca Palermo “Efficient parameter tuning for a structure-based virtual screening HPC application“. *Journal of Parallel and Distributed Computing*, Vol. 202, 15 April 2025.
DOI: <https://doi.org/10.1016/j.jpdc.2025.105087>
- JR.5. Serena Vittorio, Filippo Lunghini, Pietro Morerio, Davide Gadioli, Sergio Orlandini, Paulo Silva, Jan Martinovic, Alessandro Pedretti, Domenico Bonanni, Alessio Del Bue, Gianluca Palermo, Giulio Vistoli, Andrea R. Beccari “Addressing docking pose selection with structure-based deep learning: Recent advances, challenges and opportunities“. *Computational and Structural Biotechnology Journals*, Vol. 23, 18 May 2024.
DOI: <https://doi.org/10.1016/j.csbj.2024.05.024>
- JR.6. Bruno Guindani, Davide Gadioli, Roberto Rocco, Danilo Ardagna, Gianluca Palermo “Enabling performance portability on the LiGen drug discovery pipeline“. *Future Generation Computer Systems*, Vol. 158, 16 April 2024.
DOI: <https://doi.org/10.1016/j.future.2024.03.045>
- JR.7. Gianmarco Accordi, Davide Gadioli, Emanuele Vitali, Luigi Crisci, Biagio Cosenza, Andrea R Beccari, Gianluca Palermo “Out of Kernel Tuning and Optimizations for Portable Large Scale Docking Experiments on GPUs“. *The Journal of Supercomputing*, SI - New Trends in Parallel, Distributed, and Network-based Processing: Key Technologies, Tools, and Applications, 2 Feb 2024.
DOI: <https://doi.org/10.1007/s11227-023-05884-y>

- JR.8. Emanuele Vitali, Federico Ficarelli, Mauro Bisson, Davide Gadioli, Gianmarco Accordi, Massimiliano Fatica, Andrea R. Beccari, Gianluca Palermo “GPU-optimized Approaches to Molecular Docking-based Virtual Screening in Drug Discovery: A Comparative Analysis”. *Journal of Parallel and Distributed Computing*, Vol. 186, pp. 104819, 12 Dec 2023.
DOI: <https://doi.org/10.1016/j.jpdc.2023.104819>
- JR.9. Giulio Vistoli, Candida Manelfi, Carmine Talarico, Anna Fava, Arie Warshel, Igor V. Tetko, Rossen Apostolov, Yang Ye, Chiara Latini, Federico Ficarelli, Gianluca Palermo, Davide Gadioli, Emanuele Vitali, Gaetano Varriale, Vincenzo Pisapia, Marco Scaturro, Silvano Coletti, Daniele Gregori, Daniel Gruffat, Edgardo Leija, Sam Hessenauer, Alberto Delbianco, Marcello Allegretti and Andrea R. Beccari. “MEDIATE - MolEcular DockIng AT home. Turning collaborative simulations into therapeutic solutions”. *Expert Opinion on Drug Discovery*. Vol. 18, no. 8, pp. 821-833, 10 Jul 2023.
DOI: <https://doi.org/10.1080/17460441.2023.2221025>
- JR.10. Davide Gadioli, Emanuele Vitali, Federico Ficarelli, Chiara Latini, Candida Manelfi, Carmine Talarico, Cristina Silvano, Carlo Cavazzoni, Gianluca Palermo, and Andrea R. Beccari. “EXSCALE: An Extreme-Scale Virtual Screening Platform for Drug Discovery Targeting Polypharmacology to Fight SARS-CoV-2”. *IEEE Transactions on Emerging Topics in Computing*. Vol. 11, no. 1, pp. 170-181, 1 Jan 2023.
DOI: <https://doi.org/10.1109/TETC.2022.3187134>
- JR.11. Pedro Pinto, Joao Bispo, Joao Cardoso, Jorge Gomes Barbosa, Davide Gadioli, Gianluca Palermo, Jan Martinovic, Katerina Slaninova, Cristina Silvano “PEGASUS: Performance Engineering for Software Applications Targeting HPC Systems”. *IEEE Transactions on Software Engineering*. Vol. 48, no. 3, pp. 732-754, 1 March 2022,
DOI: <https://doi.org/10.1109/TSE.2020.3001257>.
- JR.12. Murugan, Natarajan A., Artur Podobas, Davide Gadioli, Emanuele Vitali, Gianluca Palermo, and Stefano Markidis. “A Review on Parallel Virtual Screening Softwares for High-Performance Computers”. *Pharmaceuticals*. Volume 15, no. 1: 63. 2022.
DOI: <https://doi.org/10.3390/ph15010063>
- JR.13. Roberto Rocco, Davide Gadioli, Gianluca Palermo. “Legio: fault resiliency for embarrassingly parallel MPI applications”. *The Journal of Supercomputing*. Volume 78, Issue 4, pp 2175–2195. 2022.
DOI: <https://doi.org/10.1007/s11227-021-03951-w>
- JR.14. Davide Gadioli, Gianluca Palermo, Stefano Cherubin, Emanuele Vitali, Giovanni Agosta, Candida Manelfi, Andrea R. Beccari, Carlo Cavazzoni, Nico Sanna, Cristina Silvano. “Tunable approximations to control time-to-solution in an HPC molecular docking Mini-App”. *The Journal of Supercomputing*. Volume 77, Issue 1, pp 841–869. Jan 2021.
DOI: <https://doi.org/10.1007/s11227-020-03295-x>
- JR.15. Emanuele Vitali, Davide Gadioli, Gianluca Palermo, Martin Golasowski, João Bispo, Pedro Pinto, Jan Martinovic, Katerina Slaninová, João M. P. Cardoso, Cristina Silvano “An Efficient Monte Carlo-based Probabilistic Time-Dependent Routing Calculation Targeting a Server-Side Car Navigation System”. *IEEE Transactions on Emerging Topics in Computing*. Volume 9, no. 2, pp. 1006–1019, 2021.
DOI: <https://doi.org/10.1109/TETC.2019.2919801>
- JR.16. Emanuele Vitali, Davide Gadioli, Gianluca Palermo, Andrea Beccari, Carlo Cavazzoni, Cristina Silvano. “Exploiting OpenMP and OpenACC to accelerate a geometric approach to molecular

- docking in heterogeneous HPC nodes”. *The Journal of Supercomputing*. Volume 75, Issue 7, pp 3374–3396. July 2019.
DOI: <https://doi.org/10.1007/s11227-019-02875-w>
- JR.17. Cristina Silvano, Giovanni Agosta, Andrea Bartolini, Andrea R. Beccari, Luca Benini, Loïc Besnard, João Bispo, Radim Cmar, João M. P. Cardoso, Carlo Cavazzoni, Daniele Cesarini, Stefano Cherubin, Federico Ficarelli, Davide Gadioli, Martin Golasowski, Antonio Libri, Jan Martinovic, Gianluca Palermo, Emanuele Vitali. “The ANTAREX domain specific language for high performance computing”. *Microprocessors and Microsystems – Embedded Hardware Design*. Volume 68: Pages 58-73. July 2019.
DOI: <https://doi.org/10.1016/j.micpro.2019.05.005>
- JR.18. Davide Gadioli, Emanuele Vitali, Gianluca Palermo, Cristina Silvano: mARGOT: A Dynamic Autotuning Framework for Self-Aware Approximate Computing. *IEEE Transactions on Computers*. Volume 68 Issue 5, pp. 713-728, 2019.
DOI: <https://doi.org/10.1109/TC.2018.2883597>
- JR.19. Gruttner Kim, Gorgen Ralph, Schreiner Sören, Herrera Fernando, Penil Pablo, Medina Julio, Villar Eugenio, Palermo Gianluca, Fornaciari William, Brandolese Carlo, Gadioli Davide, Vitali Emanuele, Bocchio Sara, Ceva Luca, Azzoni Paolo, Poncino Massimo, Vinco Sara, Macii Enrico, Cusenza Salvatore, Favaro John, Valencia Raul, Sander Ingo, Rosvall Kathrin, Khalilzad Nima, Quaglia Davide. “CONTREX: Design of embedded mixed-criticality CONTROL systems under consideration of EXtra-functional properties”. *Microprocessors and Microsystems* Vol. 51, 2017. pp. 39–55, ISSN: 0141-9331. DOI: 10.1016/j.micpro.2017.03.012

INTERNATIONAL BOOKS AND BOOK CHAPTERS

- BC.1. Davide Gadioli “Dynamic Application Autotuning for Self-aware Approximate Computing”. *PoliMI SpringerBriefs in Special Topics in Information Technology*, Springer 2020, ISBN 978-3-030-32094-2, pp. 91–102.

REFEREED INTERNATIONAL CONFERENCES AND WORKSHOPS

- IC.1. Roberto Sala, Nikita Litovchenko, Davide Gadioli, Gianluca Palermo, Danilo Ardagna “An Artificial Bee Colony algorithm with Machine Learning for Constrained Optimization in HPC”. *International Symposium on Modeling, Analysis and Simulation of Computer and Telecommunication Systems (MASCOTS)*. Paris, France. 2025.
- IC.2. Gianmarco Accordi, Jens Domke, Theresa Pollinger, Davide Gadioli, Gianluca Palermo “Towards High-Performance and Portable Molecular Docking on CPUs Through Vectorization”. *IEEE International Conference on Cluster Computing (CLUSTER)*. Edinburgh, Scotland. 2025.
- IC.3. Leonardo Barone, Bruno Guindani, Roberto Sala, Davide Gadioli, Danilo Ardagna, Alessandra Guglielmi “PAK-MAN: Enhancing Parallel Bayesian Optimization of Cloud and HPC Systems via Machine Learning”. *EAI International Conference on Performance Evaluation Methodologies and Tools*. Milano, Italy. 2024.
- IC.4. Gianmarco Accordi, Davide Gadioli, Giorgio Seguni, Andrea R. Beccari, Gianluca Palermo “ZS-MILES: An Approach for Efficient SMILES Storage for Random Access in Virtual Screening”. *IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*. San Francisco, USA. 2024. pp. 554-560.

- IC.5. Gianmarco Accordi, Davide Gadioli, Gianluca Palermo, Luigi Crisci, Lorenzo Carpentieri, Biagio Cosenza, Andrea R. Beccari “Unlocking performance portability on LUMI-G supercomputer: A virtual screening case study”. Proceedings of the 12th International Workshop on OpenCL and SYCL(IWOCL). Chicago, USA. 2024.
- IC.6. Lorenzo Carpentieri, Marco D’Antonio, Kaijie Fan, Luigi Crisci, Biagio Cosenza, Federico Ficarelli, Daniele Cesarini, Gianmarco Accordi, Davide Gadioli, Gianluca Palermo, Peter Thoman, Philip Salzmänn, Philipp Gschwandtner, Markus Wippler, Filippo Marchetti, Daniele Gregori, Andrea Rosario Beccari “Domain-Specific Energy Modeling for Drug Discovery and Magneto-hydrodynamics Applications”. Workshops of the International Conference on High Performance Computing Network Storage and Analysis (SC). Denver, USA. 2023. pp. 1790-1800.
- IC.7. Stefano Markidis, Davide Gadioli, Emanuele Vitali, Gianluca Palermo. “Understanding the I/O Impact on the Performance of High-Throughput Molecular Docking”. IEEE/ACM Sixth International Parallel Data Systems Workshop (PDSW), St. Louis, USA. 2021. pp. 9-14.
- IC.8. Emanuele Vitali, Davide Gadioli, Fabrizio Ferrandi and Gianluca Palermo “Parametric Throughput Oriented Large Integer Multipliers for High Level Synthesis”. In Design, Automation & Test in Europe Conference & Exhibition (DATE), Dresden, 2021.
- IC.9. Emanuele Vitali, Davide Gadioli, Andrea Beccari, Carlo Cavazzoni, Cristina Silvano, Gianluca Palermo: “An hybrid approach to accelerate a molecular docking application for virtual screening in heterogeneous nodes: POSTER”. ACM International Conference on Computing Frontiers (CF19), Alghero, Italy. 2019. pp. 298-299.
- IC.10. Cristina Silvano, Giovanni Agosta, Andrea Bartolini, Andrea R. Beccari, Luca Benini, Loïc Besnard, João Bispo, Radim Cmar, João M. P. Cardoso, Carlo Cavazzoni, Daniele Cesarini, Stefano Cherubin, Federico Ficarelli, Davide Gadioli, Martin Golasowski, Imane Lasri, Antonio Libri, Candida Manelfi, Jan Martinovic, Gianluca Palermo, Pedro Pinto, Erven Rohou, Nico Sanna, Katerina Slaninová, Emanuele Vitali: “Supporting the Scale-Up of High Performance Application to Pre-Exascale Systems: The ANTAREX Approach”. International Conference on Parallel, Distributed, and Network-Based Processing (PDP19). 2019. pp 116-123.
- IC.11. Cristina Silvano, Giovanni Agosta, Andrea Bartolini, Andrea R. Beccari, Luca Benini, Loïc Besnard, João Bispo, Radim Cmar, João M. P. Cardoso, Carlo Cavazzoni, Stefano Cherubin, Davide Gadioli, Martin Golasowski, Imane Lasri, Jan Martinovic, Gianluca Palermo, Pedro Pinto, Erven Rohou, Nico Sanna, Katerina Slaninová, Emanuele Vitali “ANTAREX: A DSL-Based Approach to Adaptively Optimizing and Enforcing Extra-Functional Properties in High Performance Computing”. International Conference on Digital System Design (DSD18). 2018. pp. 600-607.
- IC.12. Emanuele Vitali, Davide Gadioli, Gianluca Palermo, Andrea Beccari, Cristina Silvano. “Accelerating a Geometric Approach to Molecular Docking with OpenACC”. Proceedings of the 6th International Workshop on Parallelism in Bioinformatics (PBio), Barcellona Spain, 2018.
- IC.13. Cristina Silvano, Gianluca Palermo, Giovanni Agosta, Amir H. Ashouri, Davide Gadioli, Stefano Cherubin, Emanuele Vitali, Luca Benini, Andrea Bartolini, Daniele Cesarini, João M. P. Cardoso, João Bispo, Pedro Pinto, Ricardo Nobre, Erven Rohou, Loïc Besnard, Imane Lasri, Nico Sanna, Carlo Cavazzoni, Radim Cmar, Jan Martinovic, Katerina Slaninová, Martin Golasowski, Andrea R. Beccari, Candida Manelfi. “Autotuning and adaptivity in energy efficient HPC systems: the ANTAREX toolbox”. ACM International Conference on Computing Frontiers (CF18), Ischia, Italy, 2018. pp. 270–275

- IC.14. Davide Gadioli, Ricardo Nobre, Pedro Pinto, Emanuele Vitali, Amir H. Ashouri, Gianluca Palermo, Cristina Silvano and João M. P. Cardoso, “SOCRATES - A Seamless Online Compiler and System Runtime AutoTuning Framework for Energy-Aware Applications”. Design, Automation & Test in Europe Conference & Exhibition (DATE), Dresden, 2018.
- IC.15. Ahmet Erdem, Davide Gadioli, Gianluca Palermo and Cristina Silvano. “Design Space Pruning and Computational Workload Splitting for Autotuning OpenCL Applications” In RAPIDO '18 - 10th Workshop on Rapid Simulation and Performance Evaluation: Methods and Tools. p. 1-8, Manchester, UK, 2018.
- IC.16. Cristina Silvano, Giovanni Agosta, Jorge G. Barbosa, Andrea Bartolini, Andrea R. Beccari, Luca Benini, João Bispo, João M. P. Cardoso, Carlo Cavazzoni, Stefano Cherubin, Radim Cmar, Davide Gadioli, Candida Manelfi, Jan Martinovic, Ricardo Nobre, Gianluca Palermo, Martin Palkovic, Pedro Pinto, Erven Rohou, Nico Sanna, Katerina Slaninová, “The ANTAREX tool flow for monitoring and autotuning energy efficient HPC system” International Conference on Embedded Computer Systems: Architectures, Modeling, and Simulation, Samos, 2017.
- IC.17. Gorgen Ralph, Gruttner Kim, Herrera Fernando, Penil Pablo, Medina Julio, Villar Eugenio, Palermo Gianluca, Fornaciari William, Brandolese Carlo, Gadioli Davide, Bocchio Sara, Ceva Luca, Azzone Paolo, Poncino Massimo, Vinco Sara, Macii Enrico, Cusenza Salvatore, Favaro John, Valencia Raul, Sander Ingo, Rosvall Kathrin, Quaglia Davide. “CONTREX: Design of Embedded Mixed-Criticality CONTRol Systems under Consideration of EXtra-Functional Properties”. In 19th Euromicro Conference on Digital System Design, DSD 2016. p. 286-293. Limassol, Cyprus, 2016, doi: 10.1109/DSD.2016.95
- IC.18. Cristina Silvano, Giovanni Agosta, Stefano Cherubin, Davide Gadioli, Gianluca Palermo, Andrea Bartolini, Luca Benini, Jan Martinovic, Martin Palkovic, Katerina Slaninova, Joao Bispo, Joao M. P. Cardoso, Rui Abreu, Pedro Pinto, Carlo Cavazzoni, Nico Sanna, Andrea R. Beccari, Radim Cmar, Erven Rohou “The ANTAREX Approach to Autotuning and Adaptivity for Energy Efficient HPC Systems” 2016 ACM International Conference on Computing Frontiers, Como, 2016.
- IC.19. D. Gadioli, G. Palermo and C. Silvano. “Application autotuning to support runtime adaptivity in multicore architectures,” International Conference on Embedded Computer Systems: Architectures, Modeling, and Simulation (SAMOS) Samos, Greece. pp. 173-180. 2015.
- IC.20. Gadioli, D.; Libutti, S.; Massari, G.; Paone, E.; Scandale, M.; Bellasi, P.; Palermo, G.; Zaccaria, V.; Agosta, G.; Fornaciari, W.; Silvano, C., “OpenCL Application Auto-tuning and Run-Time Resource Management for Multi-core Platforms”. IEEE International Symposium on Parallel and Distributed Processing with Applications (ISPA). Milano, Italy. pp.127,133, 26-28 Aug. 2014.
- IC.21. Edoardo Paone, Gianluca Palermo, Vittorio Zaccaria, Cristina Silvano and Davide Gadioli. “Evaluating Orthogonality between Application Auto-Tuning and Run-Time Resource Management for Adaptive OpenCL Applications”. In Proceedings of ASAP 2014 - 25th IEEE International Conference on Application-specific Systems, Architectures and Processors. Zurich, Switzerland. June 2014.

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