POLITECNICO DI MILANO

PhD in INGEGNERIA DELL'INFORMAZIONE / INFORMATION TECHNOLOGY - 41st cycle

Research Area n. 1 - Computer Science and Engineering

THEMATIC Research Field: METHODS AND TOOLS FOR EXTREME-SCALE SCIENTIFIC COMPUTING ON MODERN HPC SYSTEMS

Monthly net income of PhDscholarship (max 36 months)
1600.0 In case of a change of the welfare rates during the three-year period, the amount could be modified.

Context of the research activity	
Motivation and objectives of the research in this field	The exponential growth of computational power in modern High-Performance Computing (HPC) systems enables scientific applications to tackle problems of unprecedented complexity and scale. However, this evolution also brings new challenges related to code scalability, performance portability, and efficient resource utilization across heterogeneous architectures such as GPUs and highly vectorized CPUs.The research aims to develop and optimize methods and tools for extreme-scale scientific computing, with a particular focus on applications in virtual screening for drug discovery. The main objectives are to improve performance, scalability, and portability of simulation and screening codes to fully exploit the capabilities of next-generation HPC infrastructures.
Methods and techniques that will be developed and used to carry out the research	The work will involve the design and implementation of optimization strategies for large-scale scientific applications, including: - Performance analysis and profiling on heterogeneous HPC architectures (GPUs, multi-core CPUs, vector units); - Development of scalable parallel algorithms and data management strategies; - Exploration of advanced optimization techniques based on task-based parallelism, mixed-precision computation,

	and performance-aware algorithmic design; - Use of modern programming models and frameworks ensuring performance portability (e.g., CUDA, HIP, OpenMP, SYCL, Kokkos); - Integration and testing of optimized components within the EXSCALATE virtual screening workflow; - Benchmarking and validation on state-of-the-art supercomputing systems.
Educational objectives	During the program, will be provided advanced training in HPC technologies and software engineering, scalable algorithm design, parallel programming, optimization for heterogeneous architectures, performance engineering, and scientific computing.The candidate will acquire interdisciplinary skills at the intersection of computer science, applied mathematics, and computational chemistry, enabling them to design and optimize large-scale scientific applications on cutting-edge architectures. The educational path will also strengthen teamwork, problem-solving, and scientific communication abilities.
Job opportunities	The expertise developed during the PhD will open multiple career paths in both academia and industry. Graduates will be highly qualified for positions in research institutions, pharmaceutical and biotechnology companies, and HPC centers focused on scientific computing, numerical modeling, and data-intensive applications.
Composition of the research group	2 Full Professors 0 Associated Professors 1 Assistant Professors 7 PhD Students
Name of the research directors	Prof. Gianluca Palermo, Davide Gadioli

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Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--

Housing - Out-of-town residents	--

Scholarship Increase for a period abroad	
Amount monthly	800.0 €
By number of months	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
EDUCATIONAL ACTIVITIES (purchase of study books and material, including computers, funding for participation in courses, summer schools, workshops and conferences): Financial aid is available for all PhD candidates (purchase of study books and materials, funding for participation in courses, summer schools, workshops and conferences) for a total amount of euro 6.522,20. The candidate is strongly encouraged to spend a research period abroad, joining high-level research groups in the specific PhD research topic, selected in agreement with the Supervisor. An increase in the scholarship will be applied for periods up to 6 months (approx. 800 euro/month- net amount). TEACHING ASSISTANTSHIP: availability of funding in recognition of supporting teaching activities by the PhD student. There are various forms of financial aid for activities of support to the teaching practice. The PhD student is encouraged to take part in these activities, within the limits allowed by the regulations. The availability of a COMPUTER and a DESK during the entire period of the program is guaranteed.