Politecnico di Milano

PhD in
Information Technology

Research Area n. 1 - Computer Science and Engineering

Research Title: A Bayesian Optimization approach for managing resources of High Performance Computing Systems

<table>
<thead>
<tr>
<th>Scholarships and Financial support</th>
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<tbody>
<tr>
<td>Monthly net income of PhD scholarship (max 36 months)</td>
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<tr>
<td>Increase in the scholarship for stays abroad</td>
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<tr>
<td>Number of scholarships</td>
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<td>Beginning of PhD</td>
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<td>Deadline for application</td>
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Context of the research activity

Motivations and objectives of the research in this field | Because of its strategic importance in solution of grand challenge problems and in the promotion of social and economic development, high performance computing (HPC) has been one of the most active research areas in both computer science and engineering over the last 40 years. HPC systems are complex and introduce also very complex software stacks that provide a large number of parameters influencing the final application performance. The aim of this thesis is to develop machine learning based models and a Bayesian... |
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<tr>
<th><strong>Methods and techniques that will be developed and used to carry out the research</strong></th>
<th>The techniques used and developed in this research fall under performance evaluation theory and applications, machine learning and Bayesian optimization. The research will be based on machine learning approaches applied to predict the performance of drug discovery applications and Bayesian optimization methods. The optimization final goal is to identify the minimum cost configuration of a HPC cluster which will provide performance guarantees (i.e., a deadline) for running the drug discovery simulations.</th>
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<tr>
<td><strong>Educational objectives</strong></td>
<td>From an educational point of view, the research activity aims at teaching students rigorous methods for the development of HPC systems that have strict performance requirements.</td>
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<td><strong>Job opportunities</strong></td>
<td>This research opens the doors to a career in the engineering of complex HPC systems, in particular data-intensive and scientific applications with performance concerns, in addition to an academic career.</td>
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</table>
| **Composition of the research group** | http://deepse.dei.polimi.it  
Number of Full Professors 2  
Number of Associate Professors 2  
Number of Assistant Professors 1  
Number of PhD students 1 |
| **Names of the research directors** | Danilo Ardagna |
| **Contacts** | danilo.ardagna@polimi.it  
02 2399 3514  
home.deib.polimi.it/ardagna/ |
| **List of Universities, Companies, Agencies and/or National or International Institutions that are cooperating in the research** | 1. DOMPE FARMACEUTICI SPA  
2. CINECA CONSORZIO INTERUNIVERSITARIO  
3. KUNGLIGA TEKNISKA HOEGSKOLAN  
4. UNIVERSITA DEGLI STUDI DI SALERNO  
5. UNIVERSITAET INNSBRUCK  
6. E4 COMPUTER ENGINEERING SPA  
7. CHELONIA SA  
8. TOFMOTION GMBH  
9. VSB - TECHNICAL UNIVERSITY OF OSTRAVA  
10. UNIVERSITAT BASEL |
| **Additional support** | **Educational activities** (purchase of study books and material, funding for participation in courses, summer 2\(^{nd}\) year: max 1534,00 euro per student  
3\(^{rd}\) year: max 1534,00 euro per student) |
| **Teaching assistanship:** 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. |
| **Computer availability:** | 1<sup>st</sup> year: individual use  
2<sup>nd</sup> year: individual use  
3<sup>rd</sup> year: individual use |
| **Desk availability:** | 1<sup>st</sup> year: individual use  
2<sup>nd</sup> year: individual use  
3<sup>rd</sup> year: individual use |

**Additional information**

The research will be developed within the LIGATE EURO-HPC project (GA number 956137) which aims at integrating and co-design best in class European open-source components together with proprietary (European) IPs to keep worldwide leadership on Computer Aided Drug Design solutions exploiting today high-end supercomputer and tomorrow exascale resources.