HPC4AI, an AI-on-demand federated platform endeavour

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HPC4AI, an Al-on-demand federated platform endeavour
Invited Paper

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ABSTRACT
In April 2018, under the auspices of the POR-FESR 2014-2020 pro-
gram of Italian Piedmont Region, the Turin’s Centre on High-
Performance Computing for Artificial Intelligence (HPC4AI) was fun-
ded with a capital investment of 4.5M€ and it began its deployment.
HPC4AI aims to facilitate scientific research and engineering in the areas of Artificial Intelligence and Big Data Analytics. HPC4AI will specifically focus on methods for the on-demand provisioning of AI and BDA Cloud services to the regional and national industrial community, which includes the large regional ecosystem of Small-Medium Enterprises (SMEs) active in many different sectors such as automotive, aerospace, mechatronics, manufacturing, health and agrifood.

KEYWORDS
AI-on-demand, Federated Cloud, HPC, Big Data, Fog, Industry 4.0

1 INTRODUCTION
Artificial Intelligence (AI), together with data-centric research areas such as Machine Learning (ML) and Big Data Analytics (BDA), currently represents the most valuable technological breakthrough for the Italian and European manufacturing and service sectors. It
is commonly viewed as an enabling technology for the ongoing industrial revolution, commonly referred to as Industry 4.0.

From the computer science viewpoint, the Industry 4.0 vision is outlined as an increasingly connected ecosystem of devices that produces digital data of increasing variety, volume, speed and volatility. In order to fully exploit its potential, AI applications of the next future must embrace High-Performance Computing (HPC) techniques and platforms. Secondly, computing and data management capabilities of HPC must be made readily and easily accessible on-demand to data scientists, who are more used to perform their work locally on interactive platforms.

The Turin’s Centre on High-Performance Computing for Artificial Intelligence (HPC4AI) addresses these two synergistic aspects by leveraging the skills available in two large universities and eight research institutes, federating their laboratories in a single regional centre of national importance. This new centre, equipped with state-of-the-art components of adequate size to be effective, will achieve self-sustainability thanks collaborations and business opportunities with local companies.

Over the last several years, there has been a dramatic increase in the amount data available from multiple heterogenous sources. Local companies struggle to tap the vast potential of the data deluge and gain competitive advantage through the ability to develop solutions at the forefront of research avoiding any technological lock-in by international technology conglomerates such as Google, Microsoft or Amazon. For this reason, it is necessary to create a flexible and agile research-oriented environment, inspired by a model of public-private partnership, where skills can be developed to the highest level and capable of self-sustaining through the synergy between universities, industries and SMEs.

This position paper describes the motivation, the objectives and the general structure of the HPC4AI centre.

2 MOTIVATIONS AND OBJECTIVES

General-purpose AI platforms and services are currently offered by commercial cloud providers as an integral part of their cloud portfolio. The vast majority of commercial cloud offerings have significant drawbacks with respect to the needs of an open AI-on-demand platform for the European research and industry:

- They are based on proprietary solutions that produce technological lock-in. After applications have been built, the platform will continue to exact a rent for the services deployed. The long-tail of this rental economy model increases inequalities rather than controlling them [28].
- Modern AI algorithms require specialised hardware, typically general purpose Graphical Processing Units (GPUs) or Field-Programmable Gate Array (FPGA). The cost of virtual machines that use specialized hardware is still very high in commercial public clouds; for such kind of resources, the break-even point of buying versus renting occurs quite early.
- AI and BDA algorithms work very effectively mainly on annotated datasets, which require significant human effort for curation and maintenance. Such datasets may also contain sensitive information, therefore should be stored appropriately and be compliant with European regulations if within European borders.

A cloud infrastructure dedicated to AI able to address such drawbacks should be considered a strategic asset for the regional, national and European communities.

The generation of innovative results in the field of Artificial Intelligence and Deep Learning requires performing many experiments on huge volume of data. It is also well understood that the time and the effort involved in each experiment is somehow related to the size of the training data, the characteristics of the network and the number of parameters involved. To overcome this situation, HPC4AI explicitly addresses two main technical challenges: (1) Provide AI and BDA users with an on-demand platform supporting AI and BDA solutions as services; (2) Review HPC methods and tools to meet the needs of AI and BDA.

2.1 Everything-as-a-Service by way of a Declarative Modelling Approach

HPC4AI embraces a declarative modelling approach that demonstrated its effectiveness at different levels of abstraction. A couple of examples in the direct experience of partners are the design of GARR cloud and BDA services in the Toreador project [31].

In the GARR cloud, the platform and the federation are managed and maintained through automated tools, greatly reducing the manpower required to implement a modern and efficient cloud computing platform. Automation is based on a declarative modelling approach [3] that is used to describe the structure and constraints of the cloud system components. An automation tool generates a deployment plan consisting of the steps required to achieve the requested configuration, transforming the state of the system until it satisfies all constraints. The approach offers several benefits:

- Portability: models are described in a declarative fashion, abstracting from the specifics of a cloud provider and hence they can be ported to different platforms
- Consistency: both physical and virtual infrastructures can be modelled, as well as the relationships between infrastructure, network, and application components.
- Automation: mapping a model onto infrastructure and cloud-specific deployment operations is a responsibility of the orchestrator rather than of a system administrator.

At a higher level of abstraction, methodologies to design BDA-as-a-Service (BDAaaS) based on model transformations were developed in the context of the Toreador project. Abstract declarative models are used for expressing customers’ goals and requirements in all aspects of BDA, including data representation, processing, analytics, security and privacy specification, deployment-strategy and visualisation tool definition. Such models are then converted into platform-independent procedural models specifying the desired procedures for data preparation and algorithms (including parallelisation), to be later compiled in provisioning and configuration of the computational resources on the execution platform [31].

2.2 HPC4AI, where HPC cross-pollinate AI

As digital society evolves, an increasingly connected ecosystem of devices produces more volumes and variety of data. They range from devices-in-the-fog to large and instruments addressing the grand challenges of science. To keep up with the pace, very large
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3 A FEDERATED LABORATORY

HPC4AI will be implemented as four federated laboratories connected to each other by high capacity networks. A large part of the computing and storage resources acquired within HPC4AI will be integrated into the Italian national GARR cloud federation as the “Piedmont cloud zone” [14]. By doing so, these resources will be made available to other laboratories according to a standard rate card published on the portal of the centre. Within the federation umbrella, the management of the resources of each laboratory is under the sole responsibility of the university that supplies them. This greatly simplifies the governance and the sustainability of HPC4AI since many aspects will be delegated directly to individual laboratories. The remaining computing resources will form Experimental Islands and will be available for experimentation and research within the university and wide open to project partners and external consultancy engagements. The big picture of HPC4AI is sketched in Fig. 1.

3.1 Participants

As summarized by Figure 1, HPC4AI projects has two main partners: University of Turin (UNITO) and Polytechnic University of Turin (POLITO). Each of them participates in HPC4AI contributing with different specialisations via their Interdisciplinary Centers:

- **PDF@UNITO**, the Piero della Francesca centre of UNITO, to provide AI-on-demand its applications to innovation.
- **C3S@UNITO**, the Competency Centre for Scientific Computing of UNITO, to provide a containerised distributed platform for HPC applications.
- **SmartData@POLITO**, the research centre at POLITO, to provide infrastructure and experts’ support to researchers and companies interested in Big Data and Data Science.
- **HPC@POLITO**, the Academic Computing Centre of POLITO, to provide the HPC infrastructure and technical support for academic teaching and research activities.

Several departments from the two Universities participate into the four interdisciplinary laboratories: Computer Science, Economics and Statistics, Mathematics, Law, Philosophy, Control and Computer Engineering, Electronics and Telecommunication Engineering.

To conclude, eight Technological Partners contributes into HPC4AI with their own expertise:

- **The GARR Consortium**, contributing by sharing its federated cloud software.
- **The National Institute of Nuclear Physics (INFN-TO)**, contributing by sharing its experience in designing and managing Cloud infrastructures (e.g. INDIGO-DataCloud [16]).
- **The Collegio Carlo Alberto**, contributing by sharing its experience in Economics and business models.
- **The Città della Salute e della Scienza**, which manages Turin’s hospitals, contributing by sharing its domain specialism.
- **The Human Technopole**, contributing by sharing their large datasets of medical data.
The coordination within participation and satisfaction of users. The scheme must take into account the needs and interests of the various stakeholders and different funding agencies. The coordination within bwCloud, therefore, includes the development of a solid business model and procedures that allow the participation and satisfaction of users.

The ISI Foundation, contributing by sharing its experience in Complex Systems.

The Italian Institute of Technology (IIT), contributing by starting a new HPC4AI-related laboratory on medical imaging.

The Istituto Superiore Mario Boella, contributing by sharing experience on managing large technological projects.

Figure 1: HPC4AI vision: shareholders and partnerships.

4 CLOUD FEDERATION: RELATED WORKS

Several large research infrastructures on a European scale are foreseen in the context of the ESFRI road-map [12], which aims to provide scientists adequate tools for scientific investigations. The common driver for all these initiatives is the ever-increasing demand for processing in terms of data volumes and computing power.

Seven universities in the state of Baden-Württemberg (Germany) have built federated community science cloud, through the bwCloud project [6]. The bwCloud architecture is based on OpenStack and uses a single Keystore service for authorization, while authentication is delegated to the Eduroam service among the affiliated universities. The project is focusing on a governance scheme suitable for managing a federated system that aims to support over 20,000 users. The scheme must take into account the needs and interests of the various stakeholders and different funding agencies. The coordination within bwCloud, therefore, includes the development of a solid business model and procedures that allow the participation and satisfaction of users.

SeaClouds aims to standardize management across multiple providers and to support a robust and scalable orchestration of services on them [4]. SeaClouds will intrinsically support the evolution of the systems developed with it, addressing any necessary changes, even during the execution phase. The development, monitoring and reconfiguration through SeaClouds include a unified management service, where services can be implemented, replicated and managed through harmonised standard APIs such as the CAMP specification and the Cloud4SOA project.

Apache Brooklyn is an open source framework for modelling, monitoring and managing applications for cloud environments [5]. Apache Brooklyn is able to manage the deployment of applications and prescriptions, to monitor the health and metrics of an application, to understand dependencies between components and to apply complex criteria to manage the application defined in a project.

Acumos AI Platform [30] is a federated platform for managing Artificial Intelligence and Machine Learning applications and sharing AI models, following simplicity as main design principle. AT&T has been developing the project together with the Indian consulting firm Tech Mahindra, only recently the full open source code has been made publicly available and hosted by the Linux Foundation archives. Acumos includes a standard mechanism for downloading AI code from a marketplace, bringing AI functionality to where data resides instead of requiring developers to load data into a proprietary cloud service to access AI functions.
The Nectar Cloud self-service feature allows users to access their resources coming either from commercial cloud providers or public organisations. A possible alternative is a federated approach, where the cloud infrastructure is built bottom-up by combining medium facilities into larger ones, to achieve the adequate scale [3]. HPC4AI deploy the federated GARR cloud described in Sec. 4. Cloud federation makes possible to share resources preserving the ownership, which in the case of the GARR cloud potentially embraces many Italian research institutes [14]. Likewise, since users are also owners, they are directly involved in creating and sharing services and DevOps best practices, facilitating the transition of many on-premises research activities into an off-premises cloud computing paradigm.

### 5.1.1 Services.

As described in Table 1, HPC4AI provides services that are stack of services with increasing level of abstraction: Metal, Infrastructure, Platform, BDA-as-a-Service (BDAaaS) and AI-as-a-Service (AlaaS).

The innovation potential of HPC4AI is built on four cornerstones:

- A BDAaaS/AlaaS layer specifically oriented to AI and BDA well-defined services. These services must be accessible to not tech-savvy domain experts: medical doctors, biologists, mechanical engineers, lawyers, sociologists, etc.

- A powerful and intuitive Deployment-as-a-Service (DaaS) layer from the GARR cloud layer to easily deploy complex applications in a few clicks. HPC4AI DaaS leverages on the GARR cloud that designed on top of the Juju application modelling tool and its predefined bundles of charms [18], pre-packaged recipes defining requirements and steps involved at each stage of a service lifetime. The charms to deploy Spark and Kubernetes clusters are shown in Fig. 2.

- A rich marketplace of Platforms, BDA, AI services (either for free or not) also including large datasets of specific interest for the local research community (see also the next section).

- The possibility to optimise and personalise services by moving them down to the next level of the stack and then moving them up again, e.g. to allow the optimisation or the re-training of a neural network (at the DaaS level) that is offered as a model for inference at the AlaaS level.

### 5.1.2 Datasets.

Along with the computation resources, a repository for training datasets will be provided, allowing a fast access to the data, without the need to replicate or transfer it from other sources. In addition to many publicly accessible datasets, the project will store particularly interesting datasets like:

- A mirror of the Software Heritage archive that holds over 20 million software projects, with an archive of over 2.7 billion unique source files [8].

- Labelled brain Computer Tomography scans from the Interventional Neuroradiology Unit of Molinette Hospital in Turin.

- Labelled digital histopathology slides from the Department of Medical Sciences of the University of Torino.

Collaboration between scientific and technological partners will improve and extend available datasets. For example, the Città della Salute produces hundreds of thousands of medical images per year. A significant fraction of this dataset is usable for scientific research but often cannot be moved elsewhere (e.g. public cloud) because of their size or specific restrictions (e.g. permission of use, privacy concerns, etc.). Collaboration with technological partners is also expected to make data ready to direct apply deep learning techniques, for example by improving labelling practices with respect to current standards(e.g. marking regions of interest).

### 5.2 Containerised Cloud-like HPC Platform

The C3S@UNITO Centre provides the University of Torino research community with a multi-purpose facility called OCCAM,
<table>
<thead>
<tr>
<th>Users</th>
<th>Kind of service</th>
<th>Services</th>
<th>Artifacts</th>
</tr>
</thead>
<tbody>
<tr>
<td>Application domain experts with no skills on ML and/or BDA</td>
<td>AIaaS, BDAaaS</td>
<td>AI and BDA services directly designed within HPC4AI or third parties</td>
<td>Marketplace for ML and BDA solutions, e.g. by way of AcumosAI marketplace [30]: dashboards, ML/DL models in several domains, BDA pipelines</td>
</tr>
<tr>
<td>Application domain experts skilled on ML and/or BDA but not expert in parallel and cloud computing</td>
<td>PaaS by way of Deployment-as-a-Service (DaaS)</td>
<td>PaaS solutions for ML and BDA directly designed within HPC4AI and related projects; GARR cloud DaaS</td>
<td>Marketplace of Platforms (e.g. Juju bundles) to deploy software stacks for ML and BDA; solutions for data ingestion, data lake, etc.</td>
</tr>
<tr>
<td>Researchers, cloud engineering, ML and BDA framework designers, cloud engineers, stack and automation designers</td>
<td>Infrastructure-as-a-Service (IaaS)</td>
<td>GARR federated cloud</td>
<td>Virtual Machines and networks, object storage, file storage, etc.</td>
</tr>
<tr>
<td>Researchers, cloud engineering, ML and BDA framework designers, cloud engineers, stack and automation designers</td>
<td>Metal-as-a-Service (IaaS)</td>
<td>Job scheduler for HPC resources</td>
<td>Job queue, Container orchestrators, Big Data stack (Spark, etc.)</td>
</tr>
<tr>
<td>Researchers, run-time designers</td>
<td>Hardware</td>
<td>Bare Metal</td>
<td>Multi-core CPU, GPU, storage, network</td>
</tr>
</tbody>
</table>

Table 1: HPC4AI service stack.

Figure 2: Two screenshots of the GARR cloud Deployment-as-a-Service (DaaS) interface: deployment of Spark (left) and Kubernetes (right) clusters.

with fairly conventional HPC nodes, high-memory nodes, GPUs, a high-performance parallel storage based on the Lustre filesystem [19] for data processing, and a high capacity archival storage area, with both 10 Gb/s Ethernet and 56 Gb/s InfiniBand interconnections.

The execution model on OCCAM [1] is fully based on containerisation technologies, giving the users maximum freedom in the choice of their runtime environment and, at the same time, decoupling the application software management from the infrastructure management.

A Computing Application is defined by a runtime environment (OS, libraries, software packages, services), its resource requirements (e.g. one large single-image node, HPC cluster, GPUs) and an execution model (e.g. batch jobs, pipelines, interactive access).

Linux containers provide an isolated execution environment for user software, and their use in HPC environments and, more generally, for scientific computing is currently a hot research topic.

In most cases, special tools are used to run containers in user-space on HPC nodes, such as Singularity [25] or Shifter [17]. In our case we decided to rely on Docker for container management and execution, Apache Mesos and Marathon for container scheduling [20], along with several tools and configuration templates produced by the INDIGO-DataCloud EU project [16].

Docker provides a popular ecosystem of tools for easy creation and distribution of computing applications in the form of container images, together with the availability of many off-the-shelf base images ready to use and customize. Thus, a user can develop her Computing Application container on her private workstation, then run it on OCCAM as-is or as a component in a more complex structure. Allowing users to run Docker containers natively on worker nodes poses obvious security concerns; some countermeasures were adopted to sanitise images before running them, cleaning up the attack vectors that a malicious user can leverage to break in the system security, without impacting on Docker performance or features needed to run the legitimate user tasks. Furthermore, the
users cannot access directly Docker’s APIs on worker nodes but are provided with command line interface tools that interface with Docker in a controlled way.

The choice of a containerised platform has risen from the wide range of use cases, which in turns calls for a great flexibility in the way C3S@UNITO provisions its users with resources, moving from pre-installed software packages to consolidated applications. Even though the user interfaces and work-flow are fully defined and will not change, development work is still ongoing under the hood in order to strengthen the infrastructural back-end and allow for more advanced cross-application scheduling.

All the images are stored on a private registry integrated with the main user interface provided by a repository service based on GitLab, so the users can freely manage their images, share them with other users avoiding duplication and making simulations reproducible.

5.3 HPC Platform

Founded in 2012, the HPC@POLITO Academic Computing Centre provides the HPC infrastructure inside Politecnico di Torino to many engineering research groups.

The centre directly supports a wide range of researchers coming from nine different departments, offering computing resources to scientific topics ranging from computational fluid dynamics to bioinformatics, molecular dynamics, and machine learning. Furthermore, an application engineering support is provided to help users to take advantage of the power of modern HPC systems. Individual research groups can also contribute to the improvement of the centre’s clusters by acquiring computational nodes that conform to the concurred standards.

Following the University educational mandate, HPC@POLITO also supports teaching activity such as hosting specialized programming courses of both Master and PhD students. An increasing number of students use Centre’s computing facilities to perform complex and intensive numerical simulations for their thesis. Furthermore, the number of new research activities increases year by year as well as the number of papers, published on both journals and conference proceedings, whose scientific results are obtained thanks to the computational resources made available.

All the clusters hosted by HPC@POLITO are made by distributed-memory commodity nodes interconnected by InfiniBand and sharing the same high-performance Lustre storage. The centre already hosts specialised node equipped with accelerators, whose number is expected to grow thanks to HPC4AI.

Users have the ability to create customised environments by using Singularity [25] containers. Singularity is a software container technology specifically created with the HPC use case in mind. It can be used to package entire scientific work-flows, software and data. Unlike many other container systems designed to support trusted users running trusted containers, Singularity supports the opposite model of untrusted users running untrusted containers. Images are managed through a private Singularity registry application on which HPC’s users can upload and download their images. Some pre-built images for widely used applications, for example commonly used Deep Learning frameworks like Keras or TensorFlow, are made available by the staff.

5.4 Big Data Platform

The SmartData@POLITO centre was created to target the fundamental research challenges and practical applications of big data and data science. SmartData@POLITO developed experience with big data workloads using a small-scale infrastructure, built in 2015, which is able to store around 750 TeraBytes.

The cluster has been designed to be horizontally scalable based on commodity hardware, which means that new resources can be deployed besides the existing ones, enhancing performance without impacting end users. It includes both the Hadoop distributed file systems (e.g., HDFS) and frameworks for resource management (e.g., YARN) both needed to enable general compute engines for big data (e.g., Map-Reduce and Spark).

Such infrastructure has proven instrumental for bootstrapping the centre’s activities, supporting research projects operating with dozens of TeraBytes, new collaborations with industries and Master’s Courses attended by hundreds of students annually. It is however not sufficient to explore the new possibilities offered by the combination of AI and big datasets.

HPC4AI will allow to reach new frontiers on big data processing capabilities, moving the available capacity of storing and processing data from the TeraByte to the PetaByte space.

As big data applications are increasingly relying on machine learning and AI algorithms, the SmartData@POLITO will explore novel alternatives to deploy a big data infrastructure that allows advanced AI to be executed on extremely large datasets. In terms of hardware, this will include the provisioning of infrastructure that is not only focused on provisioning large storage capacity but also compute to better handle memory-intensive workloads and the presence of specialised hardware (e.g., GPUs).

6 HPC4AI BUSINESS MODEL

Implementing a successful business model is increasingly seen as a source of innovation. Such model has to be managed in line with an organisation of business processes and strategy to become a key shaping factor for long-term sustainability [7].

Regardless of how innovation in the business model occurs, its structure [29] must enable the organisation to provide value to all its stakeholders whilst protecting its competitive position. This requires a business model that is flexible enough to allow the organisation to anticipate problems, identify and exploit opportunities, correct projects which are going astray and respond to social and technological change. For example, HPC is inextricably linked to innovation by enabling breakthroughs in science, engineering. In a business perspective, HPC is viewed as a cost-effective tool for speeding up the R&D process. HPC4AI aims to adopt a AI-centric business model which can create and defend values, seizing opportunities, able to adapt according to market needs.

For HPC4AI, we considered a model in which technologically advanced players begin to play a dual role. They are not only actors within their industry, providing value propositions to their segments of customers, but also facilitators, enabling other players within the sector to innovate their value proposition. We are planning a technology platform which provides not products or services, but an integrated business support service. However, what is less reproducible is the creation of an infrastructure that will
facilitate the company’s business (1) by promoting collaboration among key stakeholders such as suppliers, customers and producers, (2) through the creation of new opportunities by monitoring transactions and recording a high volume of information and data, and (3) by disseminating innovative trends and new technologies within different sectors.

7 CONCLUSIONS

HPC4AI starts on April 2018 with an investment of 4.5M€ and a seven years’ work plan divided into two periods: two years of design and deployment and five years of operations. In the second period, its total cost of ownership is expected to be sustained with a revenue stream coming mainly from research projects funded by several Italian/European initiatives and industrial collaborations. Beyond sustainability, it is expected as main outcome the strengthening of the scientific communities involved in this endeavor. This will be evaluated by looking at the scientific outputs of both resident scientists and their students, which ultimately embody the innovation potential of the regional and national industry.

HPC4AI is not designed to bring an immediate financial gain for partners but to support the long tail of science, allowing researchers of any discipline, without expertise in computing systems, to deploy applications readily available for production, and the researchers in computer science to master enabling technologies for the imminent Industry 4.0 revolution.

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