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## CompBioMed

**Research and Innovation Action**

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Topic: Centres of Excellence for Computing Applications

### D 5.1 Release of Community Software Repository

Work Package: 5

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Lead beneficiary for this deliverable: *UNIGE*  
Contributors: *SARA, BSC, UCL*

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<b>Dissemination Level</b>		
<b>PU</b>	Public	YES
<b>CO</b>	Confidential, only for members of the consortium (including the Commission Services)	
<b>CI</b>	Classified, as referred to in Commission Decision 2001/844/EC	

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## 1 Version Log

Version	Date	Released by	Nature of Change
V1.0	21/11/2016	Bastien Chopard	First Draft.
V1.1	23/11/2016	Bastien Chopard	Adapted according to meeting at BSC.
V1.2	12/12/2016	Bastien Chopard	Adapted according to Teleconference.
V1.3	14/12/2016	Jonas Lätt	Integrated various comments. Adapted to CompBioMed template.
V1.4	16/12/2016	Jonas Lätt	Review Version.
V1.5	21/12/2016	Jonas Lätt	Integrated various comments.
V2.0	23/12/2016	Peter Coveney	Final Version.

## 2 Contributors

Name	Institution	Role
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## 3 Acronyms and Definitions

Acronyms	Definitions
CMS	Content Management System

## 4 Introduction

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Deliverable 5.1, “Release of Community Software Repository”, accounts for the work done in Task 5.6 during months M1-M3:

Task 5.6: Create (M1-3) and Maintain (M4-M36) a Community Software Repository. Leader: UNIGE (6 PM); Partners: SARA (4), BSC (3 PM). Set up a community software repository base containing the software tools developed during the lifetime of this project. CompBioMed will create a centralized repository infrastructure, which will include, for each tool, source code (using version control software), documentation, examples and periodically run test-suites.

This deliverable comprises the present document and the actual repository, implemented on the CompBioMed web page.

It results from the work of all the partners involved in this task, namely UNIGE, SARA and BSC, but it was also discussed in a larger group, including UCL, UvA and CBK. In particular, it was discussed during the WP2 meeting at BSC, on Nov 14, 2016, and through email exchanges and WP5 teleconferences.

The present document describes the created product which, according to a decision of the participating partners, is now called “The CompBioMed Hub”, instead of “Community Software Repository”.

## 5 Activities Carried Out

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The CompBioMed Hub has been implemented within the project website, based on the Wordpress CMS. It can be visited by selecting the menu item “CompBioMed Hub” on the website [www.compbiomed.eu](http://www.compbiomed.eu). Its structure and content may evolve during the project if the community requires additional or different functionalities.

The Hub addresses the needs of two communities:

- The computational biomedicine research community, which can use the Hub to access the resources developed, centralized, and coordinated by the CompBioMed project.
- An internal network of CompBioMed partners and selected users invoking the Hub to find assistance for software development and deployment tasks within CompBioMed. Password protection is used to restrict corresponding resources to entitled users.

The CompBioMed Hub does not host any software, but only provides a link to software repositories. This decision has been taken because popular software repositories like GitHub<sup>1)</sup> offer all of the desired functionality to host software. There exists therefore no need to develop a similar infrastructure. In addition, linking to the projects, instead of hosting a copy, guarantees up-to-date version control and avoids redundancy that would be confusing to potential users.

CompBioMed considers two approaches to the community codes. In the “plug and play” approach, access to a supercomputer running a given application is possible at a given cost (each centre can provide usage resources according to their own policies). In the “do-it-yourself kit” approach, different application codes are listed on the repository, and users can build their own combination.

The CompBioMed Hub is hosted on the CompBioMed project website and is maintained by UNIGE with the following features:

- The Hub is a repository of documentation, datasets, validation results from benchmarks, and everything else useful to the CompBioMed user community.
- Throughout the CompBioMed project, the Hub will be populated with links to all the software related to the project, through its developers and/or vendors. If the developer wants it, the related open source software can be included.
- Throughout the CompBioMed project, it will be populated with clear and documented definitions of the interfaces to connect components and build the project Applications Pipelines.
- As soon as this data is available, the Hub will provide thorough information on how to obtain access to the platforms where the project Applications Pipelines are deployed and ready to use, typically the CompBioMed supercomputing partners (SARA, BSC, EPCC, Bull, LRZ) or some other providers of computation cycles (such as AWS).
- It contains a centralised assistance web page connecting CompBioMed users and partners. This web page will be accessible via a login and password. It consists of a forum, a FAQ section, and a list of email addresses corresponding to the persons in charge of each component present in the Hub. Here, “partners” mean the full and associated members of the CompBioMed project. The “users” are selected persons who will get access to the assistance web page.

Submissions to the Hub are made by CompBioMed partners through an online form, protected by a login and password. Each submission is verified by a selected CompBioMed committee before being posted on the CompBioMed Hub. In case the number of submitted projects is too large to be fully treated on a case-by-case basis by the committee, the committee can choose to define formal criteria of software quality and conformity to medical practice, in order to possibly eliminate some of the projects at an early stage.

The information below is requested for a submission. Accepted projects are then listed on the Hub using the same structure.

- A free text description explaining the purpose of the codes
- Links to scientific articles and documentation

- Programming language, software dependencies
- Type of software license
- Performance and HPC profile (e.g. scalability), required hardware, indication on which supercomputer the code runs or has been tested. Examples of submission scripts (if adequate)
- A detailed description of the input and output relevant to the Application Pipeline. This is especially important in order to be able to couple different items of software
- Links to a set of benchmark and examples
- Information regarding the level of clinical validation
- Download instructions and/or redirection to the original software source

## 6 Conclusions

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The requirements of Deliverable 5.1, “Release of Community Software Repository”, have been successfully met. In particular,

- The purpose, content, and layout of the Community Software Repository have been specified in detail and in agreement with all participating CompBioMed partners. Based on these discussions, the Community Software Repository has been renamed as the “CompBioMed Hub”.
- The CompBioMed Hub has been implemented on the CompBioMed web page.
- Two following software projects have been added to the CompBioMed Hub: The Alya software developed by BSC and the Palabos software developed by UNIGE.

In successive stages of CompBioMed, the CompBioMed Hub will be populated with further projects. Information about the usage of the software, including deployment on specific platforms, and the usage of the project’s Application Pipelines, will be added when available.

We further point out that the CompBioMed partners involved in Task 5.6 will advertise the existence of the CompBioMed Hub as widely as possible. As an example, the Virtual Physiological Human (VPH) Institute is expected to provide strong support for CompBioMed.

## 7 Bibliography / References

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- 1) GitHub: Git repository hosting service. <https://github.com>