# SILICOFCM

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**D1.2 – SILICOFCM Cloud platform**

*Version history*

| Version | Description | Date of completion |
|---------|-------------|--------------------|
| v.0.1 | Draft outline of report with initial specs from partners UL, SBG and R-Tech | 24/07/2018 |
| v.0.2 | Addition of specs from UOI and info from IIT (not available) | 13/09/2018 |
| v.0.3 | Addition of specs from BioIRC | 17/09/2018 |
| v.0.4 | Additional specs added from UOI | 18/09/2018 |
| v.0.5 | Additional info added to the report from technical partners | 28/09/2018 |
| v.0.6 | Added introductory text, conclusions, executive summary as well as info in section 'deviation from workplan' | 16/10/2018 |
| v.0.7 | Final edits including corrections of typos were made and updated info of UOI | 19/10/2018 |
| v.0.8 | Edits including BSC requirements | 26/11/2018 |
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# Executive summary

The purpose of this report is to specify hardware requirements of consortium partners who use or contribute software as part of the SILICOFCM project. The information provided in this report will be used to inform the design of the SILICOFCM infrastructure.

Based on the SILICOFCM project proposal, SBG identified seven consortium members who are using software relevant to the SILICOFCM project. SBG contacted each of the seven partners to gather hardware requirements relevant for the design of the SILICOFCM platform that will be built as part of the SILICOFCM project. Information was received from all seven technical partners. In five cases detailed information on the hardware requirements were available and are summarised in this report. In one case, detailed specification of hardware requirements was not required and is therefore marked not applicable (n.a.) in this report. In the remaining one case detailed information on hardware requirements is currently not available and is expected to be available at a later stage of the project, likely within the first 22 - 25 months. Once additional information for this one partner becomes available, the information will be gathered and (if possible) added to this report as an addendum.

The information summarised in this report will be used for the design of the SILICOFCM infrastructure and it therefore directly feeds into deliverable D1.3.

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# List of Abbreviations

| Abbreviation | Explanation |
|---|---|
| BioIRC | Bioengineering Research and Development Center |
| BSC | Barcelona Supercomputing Center |
| CPUs | Central Processing Unit |
| GiB | Gibibyte |
| GPUs | Graphics Processing Unit |
| IIT | Illinois Institute of Technology |
| MRI | Magnetic Resonance Imaging |
| MUSICO | Muscle Simulation Code |
| n.a. | Not applicable |
| SBG | Seven Bridges Genomics |
| UL | University of Ljubljana |
| UOI | Panepistimio Ioanninon |
| WP | Work package |

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# 1. Introduction

This document describes the hardware requirements for the SILICOFCM platform. Information was collected from all partners identified to require running software on the SILICOFCM platform (see section 2.1) and summarised in section 2.2. The information provided in this document is required for the design of the SILICOFCM infrastructure and therefore closely related to deliverable D1.3.

# 2. Platform Specifications

As part of Task 1.2 SILICOFCM Specification under WP1, SBG collected information regarding SILICOFCM platform requirements.

SBG started an initial email thread asking project participants to provide hardware requirements of the components developed by their institution, including CPU, GPU, RAM, disk storage, or any other specific requirement of participant components. The goal of this task is to specify hardware requirements for each component of the finalized SILICOFCM platform, so participants should exclude resources required for component development.

Participants were asked to take into consideration input file sizes expected in this particular project as they will affect resources required for computation. Additionally, size of outputs and intermediary files was to be taken into account as well, as these may affect disk space usage. Furthermore, future scalability and long-term data storage associated with executions of participants' components (for example, long-term storage of outputs, archiving of inputs or logs) should be considered

## 2.1. WPs and tasks relevant for SILICOFCM Platform Specification

From the project proposal SBG identified the following tasks (grouped by institution), which SBG believe are relevant for the SILICOFCM platform specification.

- BARCELONA SUPERCOMPUTING CENTER (BSC)
    o WP5: Task 5.2 Upgrade FE biomechanical simulation
- ILLINOIS INSTITUTE OF TECHNOLOGY (IIT):
    o WP5: Task 5.1 Upgrade MUSICO platform
- UNIVERZA V LJUBLJANI (UL):
    o WP4: Task 4.4 Development of Cardiomyopathy Risk Stratification System
    o WP6: Task 6.3 Predictive modeling using data mining algorithms
    o WP6: Task 6.4 Testing, evaluation, model validation and optimization
- R-Tech:
    o WP7: Task 7.4 Multi-Criteria Decision Making (MCDM)
- PANEPISTIMIO IOANNINON (UOI):
    o WP6: Task 6.1 Development of virtual patients models repository
    o WP6: Task 6.2 Generation and visualization of virtual heart FCM cohorts
    o WP7: Task 7.1 Integration in the cloud platform
    o WP7: Task 7.3 Refinement
- BIOIRC:
    o WP7: Task 7.2 Design and implement standard interconnection between systems
- SEVEN BRIDGES (SBG):
    o WP4: Task 4.2 Development of the bioinformatics processing pipeline for the targeted sequencing panel
    o WP4: Task 4.3 Development of the variant annotation pipeline with the appropriate data

## 2.2. Software requirements from each identified partner

The enquiry of each institution led to the following results containing information about hardware requirements for each institution. Where information is unavailable this is indicated as well.

### 2.1.1.       Barcelona Supercomputing Center (BSC)

BSC has reported that the average requirements are dependent on the kind of problem which needs to be solved. However, as an example, BSC provided requirements for the solution for an electro-mechanics tightly coupled case of a biventricular geometry of a human heart (approximately 40 million elements) on a distributed memory cluster, with GPUs (although this is not a mandatory requirement), and a Linux-based operating system in Table 1.

**Table 1:** Software requirements from BSC

| Requirement | Specification |
|---|---|
| CPUs (cores) | 2000 |
| GPUs | N/A |
| Memory (GiB) | 1.8 per CPU |
| Storage (GiB) | 90 |
| Additional Information | Not available |

### 2.1.2.       Panepistimio Ioanninon (UOI)

UOI has provided the preliminary requirements of their components, which is summarised in Table 2.

**Table 2:** Software requirements from UOI

| Requirement | Specification |
|---|---|
| CPUs (cores) | 4  (OAUTH, 1VM) |
| | 8  (Web Server (Apache Tomcat), 1VM) |
| | 8 (Django REST API, 1VM, NginX with mod_WSGI) |
| | 8 (PostgreSQL, 1VM) |
| | 4 (File Storage, 1VM) |
| | 12 (Vpop module) |
| GPUs | Not applicable |
| | 4  (OAUTH, 1VM) |

| Memory (GiB) | 8  (Web Server (Apache Tomcat), 1VM) |
| | 8 (Django REST API, 1VM, NginX with mod_WSGI) |
| | 16 (PostgreSQL, 1VM) |
| | 8 (File Storage, 1VM) |
| | 32x12 (Vpop module) |
| Storage (GiB) | 2048 (File Storage, 1VM) |
| | 1000-2000 (Vpop module) |
| Additional Information | Not applicable |

## 2.1.3.    Univerza v Ljubljani (UL)

A summary of the requirements of UL's components can be found in Table 3.

**Table 3:** Software requirements from UL

| Requirement | Specification |
|---|---|
| CPUs (cores) | at least 8 |
| GPUs | Nvidia server enabled |
| Memory (GiB) | 256 |
| Storage (GiB) | 1024 |
| Additional Information | Intel Xeon Silver Octacore 2.10GHz<br>12GB RAM (e.g. Titan V, cost: cca 3000€) or 11GB (e.g. GTX 1080 Ti, cost: cca 1000€)) |

## 2.1.4.    R-Tech

R-Tech responded that MCDM tool is web-based and that file sizes are not an issue. An MS-SQL server database is in the background of the tool.

**Table 4:** Software requirements from R-Tech

| Requirement | Specification |
|---|---|
| CPUs (cores) | Not applicable |
| GPUs | Not applicable |
| Memory (GiB) | Not applicable |

| | |
|---|---|
| Storage (GiB) | Not applicable |
| Additional Information | Not applicable |

## 2.1.5. Illinois Institute of Technology (IIT)

IIT indicated that their requirements for MUSICO and the FE multiscale solver (MEXIE) are the same as for BioIRC, which is summarised in table 5. However, IIT furthermore indicated that the software might advance further, in which case the specifications might change and IIT will provide new specifications.

**Table 5:** Software requirements from IIT

| Requirement | Specification |
|---|---|
| CPUs (cores) | 200 (MUSICO) |
| GPUs | 10x1024 (MEXIE) |
| Memory (GiB) | 1 (MUSICO) |
| | 10x12 (MEXIE) |
| Storage (GiB) | 0.5 (MUSICO) |
| | 0.1 (MEXIE) |
| Additional Information | Depending on the problem simulated MUSICO can run in few different modes: 1) simple analysis on one CPU; 2) many independent analyses simultaneously on up to 200 CPUs; 3) parallel execution of one analysis on 200-1000 CPUs. (MUSICO) |
| | This software is just for concept proofing purposes and, as a result of the project, should be replaced with a more comprehensive one. (MEXIE) |

## 2.1.6. BioIRC

BioIRC have provided the requirements of their component, which is summarised in Table 6.

**Table 6:** Software requirements from BioIRC

| Requirement | Specification |
|---|---|
| CPUs (cores) | 250-500 (X-Ray for Diffusive MRI) |
| GPUs | Not applicable |

| | |
|---|---|
| Memory (GiB) | 16-64 per core (X-Ray for Diffusive MRI) |
| Storage (GiB) | 2000-4000 in total (X-Ray for Diffusive MRI) |
| Additional Information | Although the calculations are feasible with less processors, the parameters specified are justified to provide reasonable duration of calculations. (X-Ray for Diffusive MRI) |

## 2.1.7. Seven Bridges Genomics (SBG)

The requirements of SBG's components are summarised in Table 7.

**Table 7:** Software requirements from SBG

| Requirement | Specification |
|---|---|
| CPUs (cores) | 36 |
| GPUs | Not required |
| Memory (GiB) | 60 |
| Storage (GiB) | 1024 |
| Additional Information | Not applicable |

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# 3. Deviation from the work plan

There were no changes to the work plan and the deliverable is on track for timely submission at the end of month 6 (November 2018).

# 4. Conclusions

This report summarises hardware requirements collected from each of the consortium partners who use or contribute software as part of the SILICOFCM project.

Based on the SILICOFCM project proposal SBG identified seven consortium members who are using software relevant to the SILICOFCM project. SBG contacted each of the seven partners to collect information on CPUs, GPUs, memory and storage required to run relevant software on the SILICOFCM platform as well as any additional information that may be relevant for the design of the SILICOFCM platform.

Information was received from all seven identified partners. In one case, however, detailed information on the hardware requirements is not yet available. This is the case for R-Tech.

R-Tech indicated that the MCDM tool is web-based and file sizes are not an issue. Detailed information on requirements are therefore not applicable in this case.

For all other partners, namely BioIRC, UL, UOI, BSC, and SBG all relevant information was collected and is summarised in this report.

The information summarised in this report will be used for the design of the SILICOFCM infrastructure and it therefore directly feeds into deliverable D1.3. Any additional information required for the design of the SILICOFCM infrastructure that could not be specified in this report will be gathered during the indicated time frames and added as an addendum to this report.

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