Project Acronym: MuG

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Deliverable 2.3: Plan for the Dissemination and Use of Knowledge

Lead beneficiary: Institute for Research in Biomedicine (IRB Barcelona)

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Document history

Version	Author(s)	Partner	Date	Comments
0.1	Anna Montras	IRB Barcelona	28/04/2016	First draft
0.2	Anna Montras	IRB Barcelona	03/05/2016	Second draft including minor edits. Submitted to Supervisory Board for approval
0.3	Thorsten Schneider, Andrew Yates	EMBL-EBI	13/05/2016	Revision of foreground IP section. Revision of training activities section.
1.0			17/05/2016	Approved by Supervisory Board

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Glossary

VRE: Virtual Research Environment

CoE: Center of Excellence

IPR: Intellectual Property Rights

DMP: Data Management Plan

GA: Grant Agreement

CA: Consortium Agreement

KPI: Key Performance Indicators

Executive summary

This document outlines the first version of the IPR plan of the MuG project and defines the roadmap to facilitate the engagement of the target user communities ensuring the uptake of project results (including both tools and e-infrastructure provided). To this aim, the plan for dissemination and use of knowledge targets dissemination and training activities as well as outlining the IPR management strategy and the preliminary steps undertaken to pave the way towards sustainability.

The plan will be updated accordingly as project results become available, with increasing emphasis on technology watch and sustainability of the developed virtual research environment and potential exploitation of some of the developed tools or toolboxes.

1 INTRODUCTION

The *Plan for the Dissemination and Use of Knowledge* describes the strategy of the MuG consortium in terms of management of the information assets generated by the project.

Knowledge management refers to the process of effectively identifying all the information assets related to the project and using them efficiently

- Knowledge needed by the project (Background)
- Knowledge generated by the project (Foreground)
- Definition of the strategy to manage the knowledge within the project and implementation
- Team involved in the knowledge management process

A knowledge management plan is defined hereafter that establishes the protocols for handling both the information required for the implementation of the project (background contributed by the beneficiaries) as well as the results generated from the Action, in agreement with the provisions of the Grant Agreement (GA) and the Consortium Agreement (CA).

A **dissemination action plan** is drawn, aimed at communicating the project itself as well as promoting the advances achieved in the course of the project among the target end-user communities and other stakeholders. The present document outlines the roadmap to achieve the expected objectives in terms of project impact.

The Plan for the use and dissemination of foreground and its associated KPIs will be reviewed periodically. The proficiency in following the roadmap defined hereafter and in achieving the outlined objectives will be key to pave the way for the future exploitation of results, with special emphasis on the long-term sustainability of the Virtual Research Environment for the benefit of the research community.

2 KNOWLEDGE MANAGEMENT

2.1 Types of assets and management tools

The term knowledge assets refers to any information related generated by the project:

- **Experiential assets**, i.e. skills and know-how acquired by those involved in the project. The generation of a common know-how is an essential feature in MuG, a project with a strong degree of multidisciplinarity.
- **Systematized and packaged knowledge** such as documents, specifications, manuals, databases, patents and licenses, etc.
- **Conceptual assets**: design, product concepts, etc.
- **Routine assets**, which include all the procedures established for internal operation of the consortium.

Keeping information organized and accessible by the project team in an efficient way is key for a proper knowledge management strategy. Exchange of information within the beneficiaries of the MuG project is done through the private area of the project website, which is linked to a MuG account in Basecamp, an online platform offering cloud services to store documents and files as well as management tools. As described in D1.1 (Project Handbook, section 4) Basecamp provides a suitable collaborative environment for project partners to exchange project information.

In addition, internal working groups were defined in Deliverables D1.1 (Project Handbook) and D1.2 (Quality Plan) to facilitate the daily exchange of information by topic, while regular meetings of the technical board allow interaction between work packages ensuring that efforts are harmonized within the project.

IRB Barcelona, as WP2 leader, supervises the correct implementation of the knowledge management strategy and monitors the interaction of WP2 with all work packages through the WP leaders. IRB Barcelona also administrates the MuG project website, including the private area (managed through a Basecamp account).

2.2 Access rights

The following table summarizes general rules on access rights to background and foreground as established in the Grant Agreement (Articles 25 and Article 31 respectively).

A detailed description of background contributed by each partner and specific limitations and legal restrictions that may apply in certain cases were discussed and agreed prior to the signature of the Grant Agreement. These have been exhaustively defined in the Consortium Agreement signed among the beneficiaries and have been included in the present document under section 2.3.

Table 1: General rules on access rights to background and Foreground (Grant Agreement – [1]Art. 25; [2]Art. 31).

	Access Rights to Background	Access Rights to Foreground
For project implementation	**On a Royalty-free basis as a general rule** (conditions apply as defined in the CA and in agreement with article 25.2 of the GA - see section 2.3 for details)	Partners must give each other access to results for the purpose of **implementing own tasks** under the action: **On a royalty-free basis**
For use purposes	**Under fair and reasonable conditions to be agreed** (see section 2.3)	Partners must give each other access to results for the purpose of **exploiting their own results:** **Under fair and reasonable conditions to be agreed**

Software: The general provisions for Access Rights provided for in section 9 of the CA are applicable also to Software. Parties' Access Rights to Software do not include any right to receive source or code or object code ported to a certain hardware platform or any right to receive respective Software documentation in any particular form or detail, but only as available from the Party granting the Access Rights.

2.3 Background

According to the Grant Agreement (Article 24), Background is defined as "data, know-how or information (…) that is needed to implement the Project or exploit the results.

MuG builds up on the state of the art in terms of tools available to the 3D/4D genomics community. The key pieces contributed by consortium members are described hereafter.

EXISTING TOOLS
• Tools for atomistic simulation of DNA • Tools for coarse-grain simulation of DNA and small chromatin fibers • Analysis tools of chromosome capture data • 1D web-based genome browsers • Prototypes of 3D web-based genome browsers • Nucleic Acids simulation database (BIGNASim) (MuG builds up from a prototype, which has been completed under MuG[1])

For avoidance of doubt, the specific background contributed by each one of the 6 consortium members is clearly identified in the Consortium Agreement (Attachment 1). The contributed background may be modified prior approval of the Supervisory Board. Only the background explicitly listed in the Consortium Agreement is subject to access rights obligations. In addition, specific limitations or legal restrictions to access rights regarding the listed background may apply, in agreement with article 25.2 of the grant agreement, which are clearly specified hereafter (***adapted from CA***, Attachment 1).

IRB BARCELONA

As to IRB Barcelona, it is agreed between the parties that, to the best of their knowledge, the following background is hereby identified and agreed upon for the Project. Specific limitations and/or conditions, shall be as mentioned hereunder:

Describe Background	Specific limitations and/or conditions for implementation (Article 25.2 GA)	Specific limitations and/or conditions for exploitation (Article 25.3 GA)
NaFLEX	Academic Research Only	No Commercial exploitation and non-use for own foreground exploitation
MDWEB	Academic Research Only	No Commercial exploitation and non-use for own foreground exploitation

Furthermore, the "Fundació Institut de Recerca Biomèdica (IRB BARCELONA)" excludes all background previously owned or generated by research groups other than the one directly involved in the Project or generated by the research group directly involved in the Project but outside the scope of the Project.

For the purposes of the present Project, the research group directly involved in the Project is the one led by Dr. Modesto Orozco.

BSC

As to BSC, it is agreed between the parties that, to the best of their knowledge the following background is hereby identified and agreed upon for the Project. Specific limitations and/or conditions, shall be as mentioned hereunder

[1] BIGNASim: a NoSQL database structure and analysis portal for nucleic acids simulation data.
Hospital A, Andrio P, Cugnasco C, Codo L, Becerra Y, Dans PD, Battistini F, Torres J, Goñi R, **Orozco M, Gelpí JL**. Nucleic Acids Res. 2016 Jan 4;44(D1):D272-8. doi: 10.1093/nar/gkv1301. Epub 2015 Nov 26

Describe Background	Specific limitations and/or conditions for implementation (Article 25.2 GA)	Specific limitations and/or conditions for exploitation (Article 25.3 GA)
PyCOMPSs/COMPSs	Limitations included in the Apache v2 Licence	Limitations included in the Apache v2 Licence
PMES	Limitations included in the Apache v2 Licence	Limitations included in the Apache v2 Licence

CNAG-CRG

As to CRG, it is agreed between the parties that, to the best of their knowledge , no data, know-how or information of Fundació Centre de Regulació Genòmica shall be needed by another Party for implementation of the Project (Article 25.2 GA) or exploitation of that other Party's Results (Article 25.3 GA).

CNRS

As to CNRS, it is agreed between the parties that, to the best of their knowledge CNRS grants Access Rights to all Background other than:

- All Background generated by employees, agents, representatives or students other than that generated by the research team directly involved in the Project.
- All Background generated by employees, agents or representatives that are directly involved in the Project, which is unrelated to the work plan, aims and objectives of the Project.
- All Background developed by researcher participating in the Project which is outside the scope of the Project.
- All Background which CNRS, due to existing or future Third Party rights, is unable to grant Access Rights to.

UNOT

As to UNOT, it is agreed between the parties that, to the best of their knowledge UNOT grants Access Rights to all Background other than:

- All Background generated by employees, agents, representatives or students other than that generated by the research team directly involved in the Project.
- All Background generated by employees, agents or representatives that are directly involved in the Project, which is unrelated to the work plan, aims and objectives of the Project.
- All Background developed by researcher participating in the Project which is outside the scope of the Project.
- All Background which UNOT, due to existing or future Third Party rights, is unable to grant Access Rights to.

EMBL

As to EMBL, it is agreed between the parties that, to the best of their knowledge No data, know-how or information of EMBL shall be needed by another Party for implementation of the Project (Article 25.2 Grant Agreement) or exploitation of that other Party's Results (Article 25.3 Grant Agreement).

2.4 Foreground and IP protection

2.4.1 Project results definition

MuG develops or optimizes **tools** to integrate the navigation in genomics data from sequence (1D) to 3D/4D chromatin dynamics data. The application of such tools, using the pilot projects as a reference, will lead to the generation of raw and processed **data**. MuG partners will also provide the **e-infrastructure** for the 3D/4D genomics Virtual Research Environment. The main results of the MuG project can be preliminarily summarized as follows:

1. **Scalable computational infrastructure** to support simulations on a distributed network of HPC sites, providing a new scheme for interaction between the 3D/4D genomics community and the HPC world.
    - Reference **virtual site** from which tools will be distributed and data shared.
    - **Toolbox of HPC ready software** for higher-scale simulations and for structural analysis of experimental data.
    - Scalable, high-performance **data storage** solution to store and index the different data types for analysis and visualization, and able to be efficiently queried by such tools.
    - Advanced tools for **data management**, mining and exploration.
2. **Multi-scale genome browser** allowing for the first time to connect 1D to 3D/4D genomic data and navigate across all the resolutions of DNA in the cell through a graphical user interface.
3. **Processed data** obtained as a result of the pilot projects

2.4.2 Ownership

The results generated by each partner in the framework of the MuG project will be owned by the beneficiary that generates them (or jointly by two or more beneficiaries that generate them), as established in the Grant Agreement (article 26.1).

This issue will be addressed further in M18 (D2.4-monitoring of the plan for the dissemination and use of knowledge) and in M36 (D2.5- Project Outputs). In case of results shared by more than 1 partner, the partners will proceed with the signature of a joint ownership agreement.

2.4.3 Data management

Data, including both genomic experimental data and post-processed data, is a key asset of the MuG project. The broad range of input and output data involved in the project includes genomic annotations, genome sequencing data, Hi-C data, FISH data, nucleosome positioning, 3D structures of DNA and proteins and 4D representation of biomolecule complexes.

The development and periodic revision of a Data Management Plan (DMP) is thus an essential part of the Knowledge Management strategy that has been addressed in a dedicated deliverable (**D4.2 – Data Management Plan**) under WP4 (Data Management).

The MuG DMP has been developed according to the most updated version of EC's guidelines on Data Management[2] and submitted at the end of M6, although future updates are envisaged to ensure that the DMP is in line with the latest project developments. The DMP identifies the different types of data and defines specific procedures related to data persistency, standards and curation.

[2] EC Guidelines on Data Management in Horizon 2020 (updated February 2016).
http://ec.europa.eu/research/participants/data/ref/h2020/grants_manual/hi/oa_pilot/h2020-hi-oa-data-mgt_en.pdf

As a project funded under the call "*e-infrastructures for virtual research environments* (*EINFRA-9-2015*) MuG is taking part in the H2020 Open Research Data Pilot. With the support of OpenAIRE, the pilot aims to make research data generated by selected Horizon 2020 projects accessible with as few restrictions as possible, while protecting sensitive data from inappropriate access[3]. The MuG DMP defines the data management strategy, with special care in addressing limitations that may apply in providing open access to specific data types.

2.4.4 IP Management

Any result or code obtained under the framework of the MuG funding will be reviewed is to be evaluated by technology transfer experts before publication.

The internal procedure for evaluation is described in the MuG quality plan (D1.2, section 2.1.6) and involves informing the Project Manager and providing an abstract of the results to be published in advance. IRB Barcelona will liaise with IPR experts to establish if (i) there is a value to protect IP, (ii) who holds the rights and (iii) the best approach to do so. The WP2 leader will coordinate the negotiation of potential IPR agreements with 3rd parties.

It is not clear at this early stage of the project what results will become commercially exploitable and which should be the best protection strategy. A preliminary list of potential results susceptible of becoming commercially exploitable is shown in Table 2. The information included in this table may be subject to change in the forthcoming revisions of the plan for the use and dissemination of knowledge (D2.4 and D2.5) and in the successive versions of the exploitation plan (D2.6 and D2.7).

Table 2: Potential outcomes of the project, possibilities for protection of the generated IP and exploitation. *Information in this table is tentative and not final. External consultancy services will be hired as soon as specific results become available in order to evaluate the most suitable means of protection.

Related Innovation	Project activity /WP	Result type & description	Owner(s)	Potential IP protection means*	Potential Product/ Exploitation route
Visualizer of genomic machinery with 4D resolution	**WP3**	**Software**	TBD	Copyright, confidential information, etc.	Visualization software
Optimized software modules and workflows	**WP3** **WP6**	**Software**	TBD	Copyright, etc.	Software
Models of chromatin reorganizations / Analysis of raw data and existing annotations	**WP3** **WP6** **WP7**	**Processed data**	TBD	(tbd, in agreement with DMP) ○ Data generated from public sources will be open to community. ○ Rights of data generated from private projects will remain on user's hand. ○ Agreements to be negotiated with MuG users to enhance data reuse and verification	Consultancy

[3] OpenAire - https://www.openaire.eu/opendatapilot

				(DMP to be updated accordingly).	
"Creative" database (BIGNASim DNA Simulation database)	**WP5**		Developers	Copyright [4] (tbd) Intellectual process involved in creating the scheme of the database is protected	Database
e-Infrastructure supporting the MuG VRE	**WP4, WP5**	**Computational infrastructure**	TBD	Industrial design/ Copyright / trade mark (tbd)	Software platform

3 DISSEMINATION

Dissemination activities are key in order to bring the research undertaken and the services developed to the attention of the widest possible audience, ultimately demonstrating the added-value and positive impact of the project on the European Community.

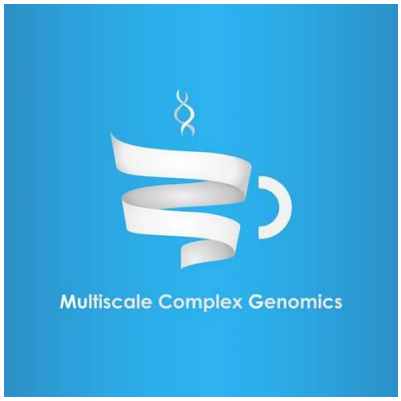
3.1 Objectives

The dissemination plan addresses the key objectives of a dissemination strategy[5]: First of all, to define the purpose of dissemination, identify the target audience and design tailored messages and partners involved, define methods and channels to reach such audiences. Secondly, to define and produce the required tools (visual identity, dissemination materials, set-up of specific platforms) to reach such audiences and last but not least, an implementation plan is needed, including timings, performance indicators and measures of monitoring the milestones of the dissemination plan.

3.2 Visual identity

Establishing a distinctive visual identity plays an important role in presenting the project to the relevant stakeholders.

The logo was designed during the first months of the project. A briefing explaining the project concept was submitted to different designers, who developed their concepts. The chosen concept is presented below:



[4] Directive 96/9/EC on protection of Databases

[5] *"Managing projects: Elaborating a Dissemination Plan"; European Commission, 2012*

Additional information on how to use the logos and project visual image is available in the project handbook (D1.1).

3.3 Dissemination strategy

3.3.1 Current situation

The first step in outlining a dissemination strategy is to define the scope of the dissemination plan. To this end, the target audiences have been identified and quantified when possible. Providing a clear picture of the state of the art in the fields addressed by the project and the advances / benefits being offered by MuG that are appealing to the target audience is key for a successful dissemination strategy.

3D/4D genomics community

The term 3D/4D genomics refers to the organization of genomes in the three-dimensional space of the nucleus. [6] This fast-growing community is facing a situation similar to that of classical (1D) genomics years ago: the community is fragmented and lacks any structure, with no consensus on analysis tools or simulation methods, disconnection between 1D and 3D/4D data, lack of standardization in data formats. This great degree of fragmentation in turn prevents the application of HPC to improve the situation.

3.3.2 Overall approach

The dissemination strategy is defined taking into account the 3 pillars of the MuG project, as shown in Figure 1. Different kinds of dissemination activities will be designed taking this in mind.

1. **Service**: MuG offers tools fitted to community needs
2. **Network**: MuG aims at engaging the community (both academic and industrial stakeholders)
3. **Joint research**: MuG aims at developing a virtual HPC infrastructure for an efficient use of computing and data resources.

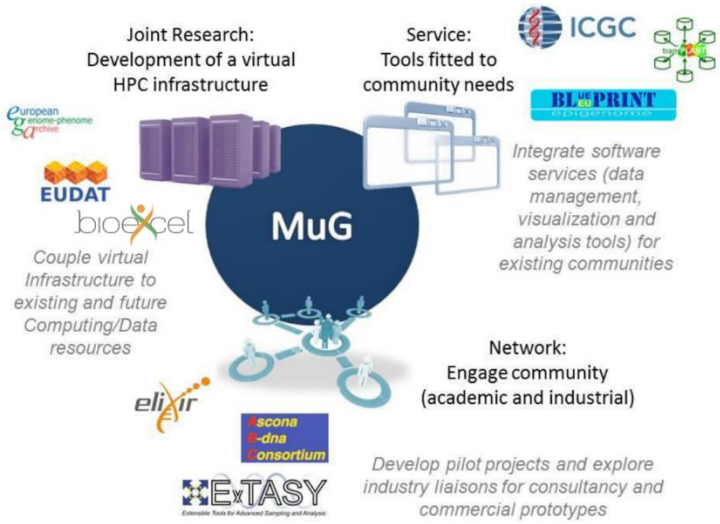


Figure 1: Mission of the MuG project

To manage interaction with the External Scientific Advisory Board (SAB), we will use the "Clientside" feature of the Basecamp account, which allows consortium members to forward specific information

[6] Martí-Renom M and Mirny L.A. (2011) Bridging the resolution gap in structural modeling of 3D genome organization. PLOS Computational Biology

via email to third parties that shall not have access to the whole contents of the private (the SAB is not a signatory of the Grant Agreement). For the purpose of information exchange with the SAB, as foreseen in the Consortium Agreement, a specific ***advisory board agreement*** will be signed, including the specifics on the information to be exchanged with the consortium and limiting the purpose of information exchange to the project.

Information to be shared publicly for dissemination purposes is regulated by the specific procedures related to dissemination and IP management

3.3.3 Key players in dissemination

IRB Barcelona, as WP2 leader, takes up the role of boosting and supervising all dissemination and training activities undertaken by all the partners and making sure that they follow a coherent strategy. Dissemination activities shall be designed according to the strategy defined hereafter, targeting specific dissemination goals and identifying the partners best suited to lead each dissemination activity.

Pilot projects play a key role in project dissemination as lead users. As such, they assume a key responsibility not only in testing the developed tools and infrastructure, but also in generating and characterizing new needs in such a way that the results will be extensible to a wider user community, that will follow on their leading path. There is a strong synergy between WP7 (pilot projects) and WP2 in the task of characterizing the user community.

3.4 Target audience's, interests and messages

3.4.1 Beneficiaries and engaging messages

The different types of stakeholders will be addressed with differentiated **messages**:

1. **The research community** is reached through publications in peer-reviewed scientific journals, participation in scientific conferences, workshops, symposia, etc. MuG is a multidisciplinary project, thus the research communities targeted by the project include several fields: general genomics, structural genomics, molecular modelling, medical genomics, computer science, etc. In addition, the achievements of MuG in terms of nucleating a 3D/4D genomics community are of general interest to the whole scientific community.
    - **Genomics and personalized medicine** research community:
        - ICGC-PCAWG
        - Blueprint
        - EGA
        - Genome England
    - **Biosimulation and 3D Genomics** community: direct beneficiaries include
        - ABC
        - ExTASY
        - HEC-BioSim
        - BioExcel CoE for computational biology:
    - **Computer Science Research community** working in HPC and Big data.

    MESSAGE: the emphasis is on the technical details of the innovations brought up by the project: (i) the MuG scalable computational infrastructure and (ii) the multi-scale genome browser.

2. **End users of the MuG Virtual Research Environment**, including stakeholders from both ***academia*** and ***industry*** (Pharma, Biotech, instrument vendors). A differentiated strategy has to be outlined to reach each target group of users:

> ***MESSAGE:*** the message will focus on how the project addresses the specific gaps and bottlenecks faced by lead-users (pilot projects) and how these are extensive to a wider community. Specific messages will be designed to tackle specific needs of end users in terms of tools, services a the tools and the infrastructure.

3. **General public** (European Society): The main objective of dissemination activities directed to the general public is to raise awareness of the benefits of MuG as an EU funded project. Activities aimed at this community involve communication with the press/audio media, talks aimed at school audiences, etc.

> ***MESSAGE:*** long term benefits of the developed infrastructure and services, including the impact that helping the research community will eventually have on accelerating the advance of, e.g. personalized medicine. Translating the technical language and to make it understandable for this kind of audience becomes an important challenge. To this end, IRB Barcelona, as coordinator and WP2 leader counts with the support of qualified staff to deal with the preparation of tailored press releases and contact with the media.

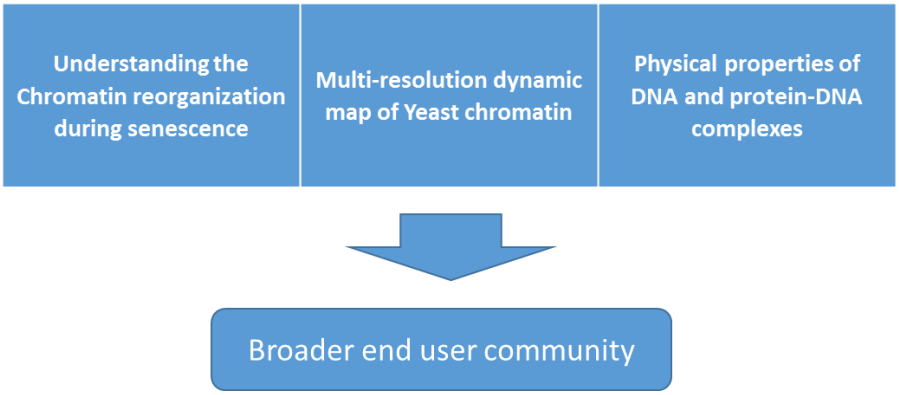
4. **EU Research infrastructure/e-infrastructures projects:** complementary initiatives have the potential of facilitating acceptance by the community, enhancing the possibility to reach a wider audience. Some some of these projects also play a key role in standardization and policy-making or offer complementary services from which MuG can benefit (or vice-versa). Securing the interaction and support of such related initiatives will be of key importance both to engage user communities and to ensure the interoperability between the services offered.
    - **HPC for Life Sciences** initiatives
        - EESI2
        - BioExcel CoE
        - CoE in Biomedicine
    - **European Infrastructures** for HPC/Big Data
        - EUDAT2020: BSC is partner. Collaboration on aspects related to the Access of data from programming models can be explored
        - PRACE: BSC is one of the main members of PRACE and the PIs of this project have been very involved in PRACE panels and are heavy users of PRACE resources. We expect a very close collaboration with PRACE, both direct and via BioExcel.
        - EGI: MuG will integrate outputs of the collaboration of BSC with EGI – e.g. COMPSs
    - **e-infrastructures projects offering complementary services, support, etc.**
        - Westlife VRE: MuG expects fluent interactions with this VRE, in the retrieval and use of experimental structural information on nucleic acids and chromatin.
        - PheNomeNal: MuG will explore collaboration with this infrastructure to integrated metabolic data in our pipelines

- BioExcel CoE for computational biology: IRB, BSC and EBI-EMBL are active partners in this CoE. Interactions with BioExcel have been initiated and are expected to be especially relevant in areas of atomistic simulations of DNA.

MESSAGE: the focus will be on synergies with the services offered by MuG and their interest for a broad research community, exploring the transversal nature of offered services and aiming at securing the long term sustainability of the MuG VRE and the interoperability with complementary services. MuG is also actively taking part in EC initiatives such as e-concertation meetings and follow-up joint initiatives such as the preparation of the e-infra booklet to disseminate the quality and promote the use of European research infrastructures browser.

3.4.2 Pilot projects as lead users

The 3 MuG pilot projects were selected as being representative of the different bottlenecks that leading researchers in different disciplines involved in this emerging community are facing. Through their leading-edge research, they generate brand-new needs that demand new and optimized tools and services in response. Therefore, pilot projects are not simply assuming a **validation role** in the project but they are acting as **lead users**, drawing the needs of an emerging community and acting as catalysts for community engagement in their respective areas, eventually leading to the nucleation of the actual community and the subsequent use of the generated tools and infrastructure.



3.5 Dissemination platforms

The different target audiences listed above will be reached using dedicated strategies that may differ from one another. Different types of **dissemination platforms** will be used to reach the different target groups according to their interests in MuG.

A summary of the differentiated strategy and the key players by area is shown in Table 3.

Table 3: Main dissemination platforms and key players in dissemination to reach different target audiences

TARGET AUDIENCE		MuG partners involved	DISSEMINATION PLATFORMS			
Type of audience	Specific community		Scientific conference / Journal	Project Website & Social media	General press	Training workshop (Expert/user)
Research community	General genomics	All	X	X		X
	Structural genomics	CNAG-CRG, IRB, UNOT	X	X		X
	Functional genomics	CNRS	X	X		X
	Molecular Modelling and dynamics simulation	IRB, UNOT, BSC	X	X		X
	Medical genomics	All	X	X		X
	HPC applications	BSC, IRB, UNOT		X	X	X
Complementary e-infrastructures initiatives (EU & local)		BSC, IRB		X		X
Manufacturers of sequencing equipment		All				X
Public health		All				X
Pharmaceutical companies		All				X
EU Society		All		X	X	

3.6 Target dissemination activities

The provisional list of dissemination activities listed hereafter have been outlined taking into account the different types of audiences and dissemination platforms identified above.

Planned dissemination and training activities include:

- Presentation of technical progress in international scientific conferences targeting the research or education community.
- Publication of results in peer-reviewed journals (see 3.6.1)
- Dissemination of project innovations and services in symposia and other events with strong presence of industry players, policy makers, complementary research e-infrastructures and other relevant stakeholders beyond the academic world.
- Dissemination of project activities in media targeting a wider public (newspapers, business magazines, etc.).
- Partners will take advantage of networking events with presence of stakeholders, meetings with collaborators, etc.
- Release of different kinds of information through the project website and social media (Twitter, YouTube, etc.) Joint dissemination initiatives related to EU e-infrastructures: participation in initiatives of the EU aimed at disseminating the excellence of European research infrastructures.

1. 11th e-concertation meeting for European e-infrastructure projects (Brussels 9th November 2015)
2. RDA plenary , February 2016 (MuG is featured alongside other funded e-infra projects)
3. Contribution to the e-infrastructures booklet

- Mailing lists and existing user communities around existing tools will be used to promote the new VRE.
- Newsletters (to be publicized through the website, partner websites, social media)

3.7 Training Activities:

- Dedicated MuG Training Workshops with the presence of keynote speakers and stakeholders on the field of genomics and 3D modeling. Two events are planned, in which training on the tools and services available through the MuG VRE will be offered
    1. EBI (2017)
    2. Barcelona (2018)
- Our workshops will be advertised on EMBL-EBI's training portal (https//www.ebi.ac.uk/training) with additional advertising on social media and local conference newsletters.
- Reach collaborations to take part in relevant workshops: We will pursue for tools offered by the MuG VRE to be incorporated in INB and EMBL-EBI own training roadshows with the aim to raise awareness in the context of general hands-on workshops. The PRACE course organized from BSC on molecular simulations is also regarded as an important platform to spread our technologies and databases in the entire bio-simulation community.Issued training materials for end users (workshops) will be made available on the website, social media or YouTube channel for the benefit of a wider audience under a CC BY-SA 4.0 license.

3.8 Target Scientific Journals and published papers

High impact publications are key to reach and engage the research community. The internal procedure for the publication of joint results generated in the framework of the MuG project is established in **section 2.1.6.1** of the MuG **Quality Plan (D1.2).** This procedure involves obtaining the consortium approval for any publication /communication and is aimed at ensuring that the exploitation potential is not jeopardized due to releasing sensitive information (as established in the Grant Agreement – articles 29.1 and 27.1).

Following H2020 rules, as soon as a publication is accepted, the obligation applies to ensure open access to publications for all beneficiaries, as stated in the grant agreement (Article 29.2). All partners of the consortium will pursue the way to publish research results funded by MuG activities with a "green" model or a "gold model".

Some results have already been published that have been (partially) developed under the MuG project. The papers published until M6 are listed below:

- Multiscale simulation of DNA.
  Dans PD, Walther J, Gómez H, **Orozco M.**
  Curr Opin Struct Biol. 2015 Dec 18;37:29-45. doi: 10.1016/j.sbi.2015.11.011.Review.

- BIGNASim: a NoSQL database structure and analysis portal for nucleic acids simulation data.
  Hospital A, Andrio P, Cugnasco C, Codo L, Becerra Y, Dans PD, Battistini F, Torres J, Goñi R, **Orozco M, Gelpí JL**.
  Nucleic Acids Res. 2016 Jan 4;44(D1):D272-8. doi: 10.1093/nar/gkv1301. Epub 2015 Nov 26.

- Long-timescale dynamics of the Drew-Dickerson dodecamer.
  Dans PD, Danilāne L, Ivani I, Dršata T, Lankaš F, Hospital A, Walther J, Pujagut RI, Battistini F, **Gelpí JL**, Lavery R, **Orozco M**.
  Nucleic Acids Res. 2016 Apr 15. pii: gkw264. [Epub ahead of print]

The following list, contains a compilation of relevant journals commonly used by the different partners in their respective fields of research. The publisher and the open access model for each journal are included.

Table 4: Common peer-reviewed journals for MuG consortium partners

Journal Title
Advances and Applications in Bioinformatics and Chemistry
Bioinformatics
Briefings in Functional Genomics
Current Opinion in Cell Biology
Current Opinion in Genetics & Development
Current Opinion in Structural Biology
European Biophysics Journal
Current Bioinformatics
FEBS Letters
Genome Biology
Genes & Development
Journal of Chemical Theory and Computation
Journal of the American Chemical Society
Journal of Molecular Biology
Methods in Molecular Biology
Molecular Cell
Nature Structural & Molecular Biology
Nature Biotechnology
Nature Methods
Nature Genetics
Nature Reviews Genetics
Nature Reviews. Molecular Cell Biology
Nucleic Acids Research
PLoS Computational Biology
PLoS Genetics
Structure
Trends in Genetics

3.9 Scientific conferences and related worskshops

Target events include but are not limited to scientific conferences involving any of the different scientific and technical disciplined involved in MuG.

The role of participating in scientific conferences is two-fold: (i) to disseminate project results, (ii) networking with the scientific 3D/4D genomics community, i.e. the end users of the MuG VRE.

Target dissemination events for the first 2 years of the project, as well as regular events organized periodically have been listed and will be periodically updated.

A dissemination events list is kept on basecamp, accessible to all partners to edit and view. https://3.basecamp.com/3126297/buckets/97795/google_documents/51087509

Table 5: Target events (workshops, conferences) for MuG-related developers, end users and other relevant stakeholders. (*) key events to reach broad end user community.

Event description	Date	Location	Organizer	Attendees
11th e-concertation meeting for European e-infrastructure projects	9/11/2015	Brussels	European Commission	IRB Barcelona BSC
PATC Course: Programming Distributed Computing Platforms with COMPSs	4/2/2016	BSC , Barcelona, Spain	PATC	BSC, IRB
Models for Protein Dynamics 1976-2016	15/02/2016	CECAM-HQ-EPFL, Lausanne, Switzerland	CECAM (Centre Européen de Calcul Atomique et Moleculaire)	Modesto Orozco (IRB)
Ciclo Conferencias Universidad de Murcia	3/3/2016	Aula Magna de la Facultad de Veterinaria, Universidad de Murcia	Facultad de Biología, Universidad de Murcia	Modesto Orozco (IRB)
VizBi2016	9/3/2016	EMBL Heidelberg, Germany.	http://vizbi.org/2016/Organizers/	CNAG-CRG (Mike Goodstadt)
Joint meeting of the Italian systems biology and epigenetic networks (SYSBIO-EPIGEN joint workshop - Epigenetics and Systems Biology)	11/3/2016	University of Milano – Bicocca (Italy)	SYSBIO Centre of Systems Biology / Sapienza University of Rome & EPIGEN Coordinator	Modesto Orozco (IRB)
Chromatin and Epigenetics (C2)	20/03/2016	Whistler, British Columbia, Canada	Keystone Symposia	CNRS (Giacomo Cavalli)
Barcelona Data Science Meeting	21/03/2016	Universitat Pompeu Fabra (Barcelona, Spain)	Barcelona GSE (Graduate School of Economics) + UPF	Modesto Orozco (IRB)
IWBBIO 2016: 4th international work-conference on bioinformatics and biomedical engineering	20/4/2016	Granada, Spain		IRB
Bioinformatics: Challenges and Opportunities in the Horizon Framework / XIII Symposium on Bioinformatics	10/5/2016	Vera Campus / Universidad Politécnica de Valencia (Spain)		IRB (Adam Hospital) BSC (Josep Lluís Gelpí)
ISC High Performance 2016	19/6/2016	Frankfurt, Germany	ISC Team	BSC

"Genome Architecture in Space and Time"	20/6/2016	Trieste (Italy)	International centre for Theoretical Physics (ICTP)	CNAG-CRG
"Theory and Simulation Across Scales in Molecular Science"	24/07/2016	Girona, Spain	Computational Chemistry. Gordon Research Conference	IRB Barcelona (Speaker: Modesto Orozco)
NII Shonan Meeting "Web-based Molecular Graphics"	5/9/2016	Shonan Village Center, Japan	http://shonan.nii.ac.jp/seminar/seminardetails086/	Mike Goodstadt (CNAG-CRG)
MGMS - "Big Data in Biomolecular Systems"	9/9/2016	School of Pharmacy, UCL, London	https://bigdatamgms.wordpress.com/#post-33	tbc
Big Data in Biology and Health - EMBL-WELLCOME genome campus conference	25/09/2016	EMBL Heidelberg, Germany.	EMBL	
BioData World Congress 2016	26/10/2016	Wellcome Genome Campus; Cambridge (UK)		
From Functional Genomics to Systems Biology	12/11/2016	EMBL Heidelberg, Germany.	EMBO	
SuperComputing 2016	13/11/2016	Salt Lake City, Utah	SC Commitee	BSC
From genomes to structures: looking at big data with an atomic perspective	28/11/2016	Barcelona, Spain	IRB Barcelona (support BBVA foundation)	I
Architecture and plasticity of the cell nucleus	29/11/2016	Paris, France	Giacomo Cavalli	IGH-CNRS
(*)**EMBO Conference Series on Nuclear Structure and Dynamics 2017**	2017 (date tbc)	France		IGH-CNRS, CNAG-CRG
(*)**Nuclear Organization and Function meeting (Cold Spring Harbor) 2018**	2018 (date tbc)	Cold Spring Harbor (NY, USA)		IGH-CNRS, CNAG-CRG
TADbit yearly training events			CNAG-CR G	
EGI Conferences/Community Forums			EGI	
BioExcel workshops and webinars			BioExcel	

3.10 Dissemination materials

3.10.1 Project brochure

The project brochure). Taking advantage of the preparation of the contents for the project factsheet, a project brochure was designed at M3 (D2.1 - Project Factsheet). The final version of the brochure is now available for download from the project website and is included in Annex I.

Status: Complete
Download link: http://www.multiscalegenomics.eu/docs/MuG_Factsheet.pdf

3.10.2 Project Poster

A project poster is on the works at the time of preparation of this report. The brochure targets a broad audience, bringing to the attention of both the general public and the target end users the benefits of the project and acknowledging the EU funds.

The new poster will contain more advanced technical content, focusing on the needs of different end user target groups who can benefit of the project outcome.

- Status: Underway
- Timings/ action list:.
    - M7 (May 2016): A first version of the poster will be released on 10/05/2016 at the JBI 2016 (XIII Symposium in Bioinformatics) in Valencia. The postar will contain general information about the project and its benefits for the overall 3D/4D genomics community.
    - M12+: Upgraded poster (or different versions of the poster) targeting specific audiences and containing higher technical detail and project results will be designed as the project progresses and more results become available. WP2 will coordinate with WP6/WP7 in the task of characterizing the needs and defining a clear differentiated message for each user.

3.11 Communication strategy

Press and media involvement are essential in order to raise awareness among the widest possible audience, to ensure that the information flow is not limited to the circle of influence of the project beneficiaries and reaches all relevant stakeholders required to validate the need for a sustainable community and infrastructure in the long term.

The consortium has the support of local press offices of the partner institutions, which contribute to achieving the maximum impact in the media, both at national and international level by informing news agencies, printed mass media outlets, televisions, radios and digital media about relevant events related to the project (e.g. training workshops, annual meetings, high impact publications, etc.).

As a first step, an initial press release was issued on the date of the project kick-off-meeting, in December 2015. The text of the press release and examples of media coverage of this press release has been collected in Annex II.

3.12 Project website

The design and contents of the MuG project website have been described in detail in the dedicated deliverable 2.2. The project website is progressively increasing its features and an upgraded version with improved functionality is on the works.

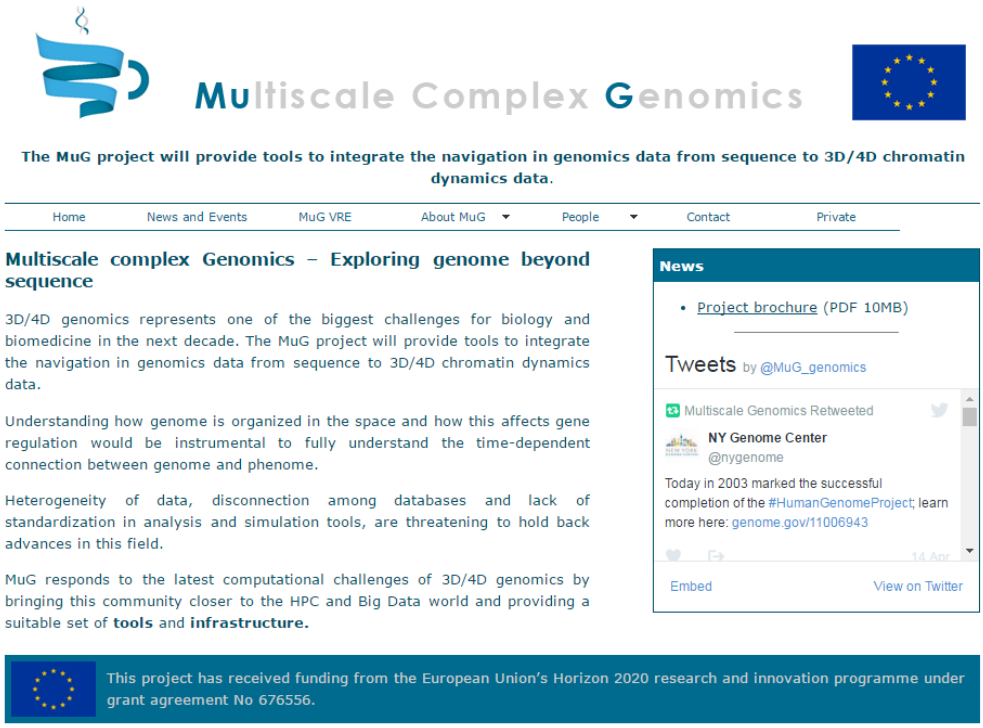
- Status: Online M2. Ongoing
- Action Plan: a full upgrade of the dissemination website is needed as well as the development of the VRE portal.

  M7-M8: Release of improved website, with increased functionality and features of the dissemination website

  M18: VRE portal preliminary version

  M36: VRE portal full functionality

The current version of the website is shown in the following figures:



3.13 Newsletters

The project has foreseen to issue a periodic newsletter with information about the latest developments and upcoming activities related to MuG.

The release of the first newsletter is foreseen to take place in parallel with celebration of the M6 general meeting. The newsletter will be issued periodically.

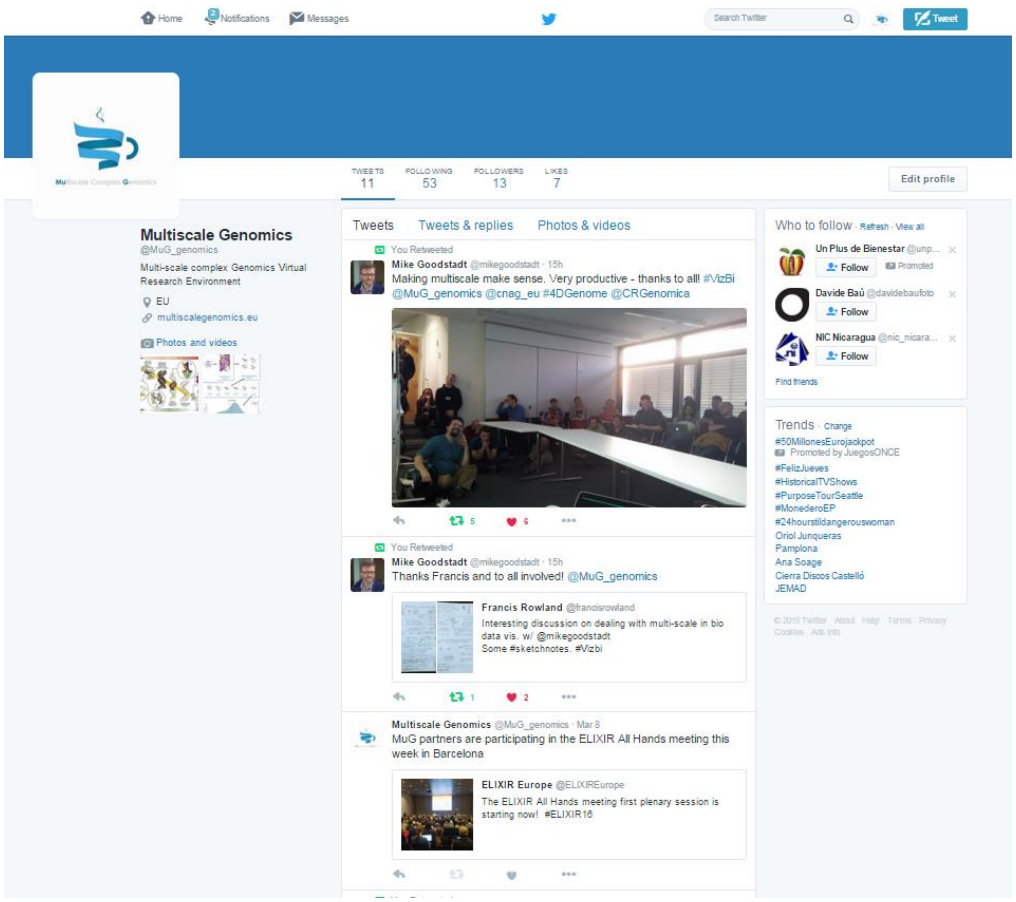
- Status: Underway
- Action Plan:
  - M6: Call for contents of future newsletters
  - M8: Foreseen publication of the first newsletter (foreseen periodicity: 6 months)

3.13.1 Social media tools

Social media networks will be used with the aim to increase the visibility of MuG developments, creating a network that reaches all relevant stakeholders.

A Twitter account has already been set-up and embedded in the project website. Twitter is a good platform to keep updated about activities in the radar of MuG undertaken by relevant stakeholders and is a good starting point to open up networking possibilities and expand the contact network beyond the usual circle of partners and collaborators.

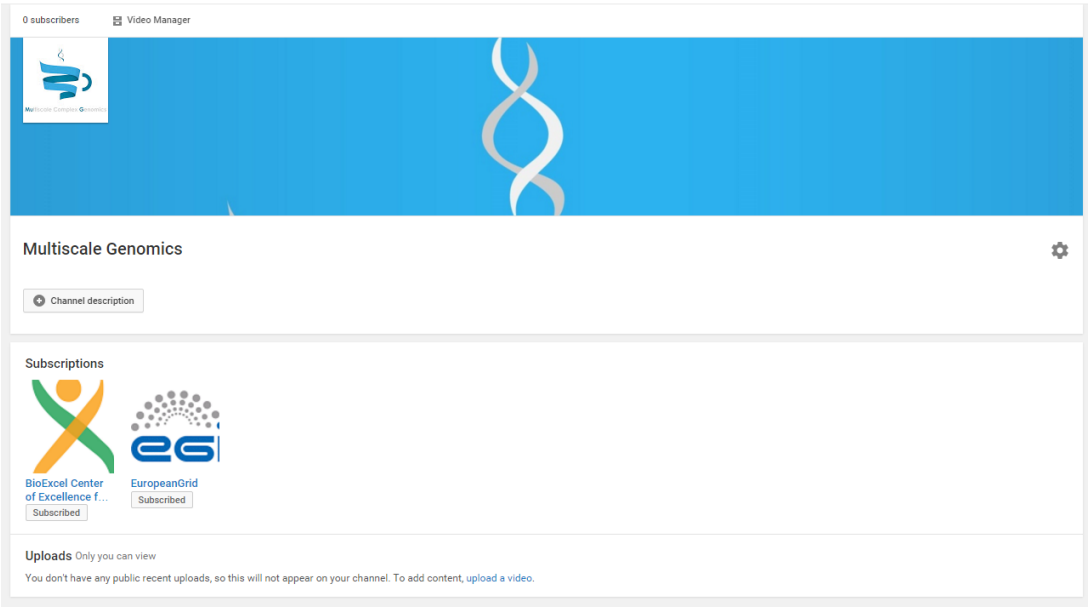
Other social networks will be considered in the future, such as LinkedIn to boost contacts with Industry.



3.14 YouTube channel

Will be useful for future hosting of training videos, etc. related to the MuG VRE, which can be linked from the project website.

The channel has already been set up and is ready to upload contents.



4 KEY PERFORMANCE INDICATORS

Key performance refers to the way in which the project knowledge assets should be managed in order to maximize the performance. The first step will thus be the definition of the project performance objectives, which are defined taking into account the needs of the different stakeholders that will benefit from the project (research community, European research infrastructures, industrial end users, etc.). The performance objectives are translated into a number of performance indicators that allow to measure performance achievement.

The success, in terms of reaching the target communities, of dissemination and training activities as well as the feedback received from participants, allows us to measure the performance of the project.

4.1 KPIs, metrics and timing

The KPIs allowing us to monitor the impact of the project were outlined in D1.2 (quality plan) and are listed hereafter. Periodic monitoring of the KPI metrics will allow us to identify the aspects of the project that need to be revised in order to improve these figures.

KPI and metrics description	Metrics description	Target 2016	Target 2017 (cumulative)	Target 2018 (cumulative)
Interest of companies to collaborate with MuG.	Number of contacts established with industry: • Pharma • Biotech • Instrument vendors	1	3	10
Presence in the media	Number of published news reports.	5	15	30
Scientific publications	Number of publications in top-ranked scientific journals	3	6	12
Citations	Number of citations in top-ranked scientific journals	n.a.	n.a.	We expect to collect citations in top-ranked journals during the last year of the project.
Presence in International congresses	Number of events where MuG results are presented	5	10	10
Attendees in training workshops (indirect measure of users reached, together with	Number of attendees in two workshops (2017 and 2018). A significant increase is expected due to (i) dissemination plan, (ii) quality of VRE services.	0	30	70

VRE portal usage)				
Project website functionality and performance	• Implemented means of improving performance • Implemented new features • Frequence of updates • Cross links to and from other websites in the fied. • Google analytics statistics	• Communication / dissemination functionality. implemented. • Weekly updates.	• Updated web. • MuG VRE portal. implemented. • increasing visitors.	• MuG VRE portal fully operational. • Increasing visitors.
Impact on social media (twitter, youTube)	No twitter followers No videos on YouTube No subscribers YouTube	50 2 10	100 10 50	150 15 100
Generation of commercial prototype projects	No commercial prototype projects.	0	0	At least 1 prototype with a third party SME.
Candidate technologies for IPR protection	Number of evaluated technologies Number of protected technologies	0 0	1 0	2 1

4.2 KPI monitoring

The monitoring procedure for the KPIs is defined in D1.2 (Quality Plan) – section 3.1.1- and is reproduced hereafter for ease of reference:

- The degree of achievement of the KPIs shall be a regular activity to be undertaken by WP leaders. KPIs, together with risks, should be addressed in monthly Technical Board meetings.
- During regular meetings of the Supervisory Board (every 6 months) the status of KPIs shall be assessed.
- The Supervisory Board may at any time consult with the Scientific Advisory Board regarding possible measures that could be undertaken to increase performance for the different indicators.
- Assessment of the KPIs will also be one of the key points in the agenda during SAB yearly meetings.
- A live table of KPIs will be maintained in BaseCamp for easy monitoring by all partners.

5 SUSTAINABILITY ROADMAP

MuG must be sustainable beyond the 3-years grant period. Efforts undertaken in the 3-year project to develop excellent quality tools and infrastructure need to be backed by the right strategy to reach the user communities and engage them in embracing the use of such optimized tools.

3D/4D genomics is in its early stage of development but the community is already large and has been growing exponentially for the last 5-10 years. Two of the main meetings of the community (Nuclear Organization and Function meeting at Cold Spring Harbor and the EMBO conference series on Nuclear Structure and Dynamics) gather around 300 scientists. Other meetings focused in more specific aspects of the broader 3D/4D genomics field have allowed us to estimate that, altogether, **more than 3000 researchers** are currently working in this field. At the current growth rate, motivated by the advent of experimental techniques, such as Hi-C, to study chromosome folding, we expect a high demand for the services offered by MuG.

The involvement in MuG of two leading service-provider centers (EMBL-EBI and BSC) will certainly facilitate the long-term sustainability of MuG. The main pillars on which the project is built are (i) Excellence in tools, (ii) Excellence in infrastructure and (iii) Excellence in user engagement. User engagement can only be achieved through a right dissemination and outreach strategy, which involves ensuring that the impact goes far beyond the circles of influence of the 6 project partners.

The dissemination of project results, essentially the results and feedback obtained from the **pilot projects**, as well as the training workshops on the use of tools, will be key in paving the way towards the sustainability of the Virtual Research Environment.

Work Package 6 (Analysis tools) and WP7 (pilot projects) are working together since day 1 to ensure that the developed tools respond to actual needs of the users. During the first months of the project, a thorough evaluation of the analysis tasks performed by the pilot projects, their demands and the current tools available has been performed.

As a result of this first internal exercise it will be possible to perform a first evaluation of the state of the art of analysis tools, identifying gaps and potential for improvement. The consultation will be extended to a broader user community (beyond the consortium pilot projects) in the following stage in coordination between WP2, WP6 and WP7. This consultation shall be performed by means of a **user**

survey. The survey will be made available online and announced to relevant users both in academia and industry through mailing campaigns or in relevant dissemination events (conferences, symposia, etc.). The survey will validate the outcomes of the exercise undertaken by analysis tools providers and pilot projects, giving very relevant information about the needs of a wider community and representing a first step in articulating a virtual community.

Discussions regarding the measures to be taken in order to materialize the eventual transition from ***Project*** to an ***Infrastructure*** (robust and reliable in the long-term) have started and will become a priority in the next months.

It is expected that following the end of the project in 2018, a TRL of 7 to 8 is reached, which should be followed by a consolidation phase and eventually evolve to a permanent infrastructure (TRL9) with a stable financial sustainability. To this end, MuG relies on the following supports:

1. **European support initiatives**. This is the simplest and most robust mechanism to provide long-term sustainability to MuG:
    - PRACE and EUDAT: BSC is partner in both initiatives. MuG will be benchmarked on Marenostrum (PRACE Tier 0) and will use B2SAFE EUDAT service (which is already supporting the ABC consortium)
    - HPC CoEs in Life Science (e.g. BioExcel) in which EMBL- EBI, IRB and BSC participate, are excellent partners to guarantee the long-term sustainability of our developments.
2. As part of our strategy, **MuG services will be also part of the catalog of the National Institute of Bioinformatics** (BSC, CNAG-CRG, and IRB are three nodes of the INB), the European Bioinformatics Institute and ELIXIR (EMBL- EBI, BSC and IRB are full partners of ELIXIR). ELIXIR has expressed its interest (and the Spanish node its full commitment) in the long-term support of our infrastructure (if successfully developed).
3. **Support international genomics initiatives**. MuG aims to be a reference platform in the field of genomics and personalized medicine. Starting with the pilot projects (WP7) we will work towards the integration of the platform to existing international initiatives (ICGC, Blueprint, etc.) that explicitly support the development of the MuG VRE. Once MuG is deployed, we will reach agreements with those initiatives to co-fund MuG services.
4. **Industry supports** will be pursued through WP2 activities with the aim of turning MuG innovations into exploitable results and consultancy. Genomics is an exciting field for industry, start-ups and venture capital. IRB and BSC's technology transfer officesthe development of the business plan and supporting MuG-Industry liaison.
5. **Potential EU funding for consolidation and integration of e-infra platforms** under the 2018-2020 Work Programme would facilitate the needed transition to TRL9.

The first outcomes of consortium internal discussions, potential contacts initiated with external stakeholders (other research infrastructures, industry, etc.) will be reported in M18 in the Initial Exploitation Plan (D2.6).

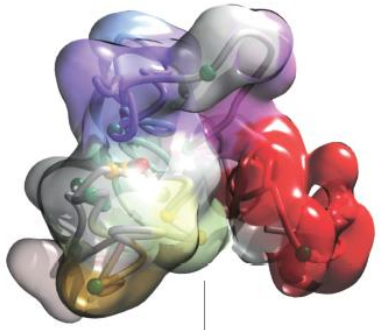
6 ANNEX I: PROJECT BROCHURE

EXPLORING GENOME **BEYOND SEQUENCE**

3D and 4D genomics represent one of the greatest challenges for biology and biomedicine in the next decade.

Research efforts in 3D and 4D genomics are experiencing exponential growth. However, the current lack of standardization in analysis and simulation tools is threatening to become a bottleneck. MuG responds to the latest computational challenges of 3D/4D genomics by bringing this community closer to the HPC world and providing a suitable set of tools and infrastructure.

Understanding how genome is organized in the space and how this affects gene regulation would be instrumental to fully understand the time-dependent connection between genome and phenome.



3D REPRESENTATION OF A HUMAN DNA FRAGMENT
(COPYRIGHT: MARC MARTÍ-RENOM, CNAG-CRG)

Multiscale Complex Genomics

Coordinator: Dr. Modesto Orozco (IRB Barcelona)
Start date: 1st November 2015
Project duration: 36 months
EC contribution: 2.961.163,00 €
Project website: www.multiscalegenomics.eu

Coordinator

IRB BARCELONA
INSTITUTE FOR RESEARCH IN BIOMEDICINE

Partners

Barcelona Supercomputing Center · EMBL · cnag · cnrs · The University of Nottingham

EXCELENCIA SEVERO OCHOA

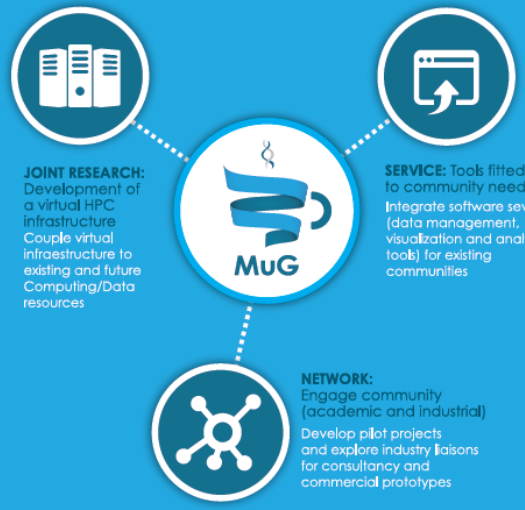
IRB Barcelona, BSC and CNAG-CRG have been awarded the "Severo Ochoa center of excellence accreditation" by the Spanish government in recognition of their outstanding performance in the international research arena.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 676556.

BRINGING SCIENCE AND TECHNOLOGY CLOSER

The vision of the MuG project lays on the achievement of the following challenges:

- **To prevent a potential collapse** in 3D/4D genomics due to inability to manage the computational problems originated by massive sequencing experiments and simulations.
- **To nucleate the 3D/4D community** and bring it closer to the HPC and Big Data world.
- To provide an **integrated three-dimensional picture of the genome.**



JOINT RESEARCH: Development of a virtual HPC infrastructure Couple virtual infraestructure to existing and future Computing/Data resources

SERVICE: Tools fitted to community needs. Integrate software sevice (data management, visualization and analysis tools) for existing communities

NETWORK: Engage community (academic and industrial)

Develop pilot projects and explore industry liaisons for consultancy and commercial prototypes

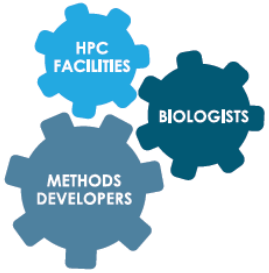
KEY INNOVATIONS

A scalable computational infrastructure for multi-scale complex genomics, defining a new scheme for interaction between the 3D/4D genomics community and the HPC world

Modelling of chromatin re-organizations aimed at improving the knowledge on cell biology and predicting links to disease.

Connect 1D to 3D/4D genomics data, allowing for the first time to navigate across data from different sources and scales in a single "complex" model.

Visualization of complex genomic machinery with a 4D multiresolution picture.



WORLD LEADING EXPERTS

A high-profile, multidisciplinary consortium:

IRB Barcelona (Modesto Orozco, Coordinator): Developer of the most used tools for analysis and simulation of nucleosome fibers. Expertise in developing tools for high-resolution DNA simulation; Analysis of DNA physical properties;

BSC-CNS-Life Sciences (Josep Ll. Gelpí) and Computer Sciences (Rosa M. Badia) departments: Supercomputing centre with large experience in supporting bio-HPC problems. Broad experience in modelling protein-protein and protein-nucleic acid complexes.

CNAG-CRG (Marc Marti-Renom): World-leading activity in developing approach for reconstructing chromatin structure from Hi-C data.

CNRS-IGH (Giacomo Cavalli): one of the most active groups in connecting chromatin structure with cell behaviour.

University of Nottingham (Charles Laughton): Expertise in developing tools for high-resolution DNA simulation and with large experience in analysis of DNA physical properties.

EMBL-EBI (Andrew Yates): World-leading group in genomics data management.

USER DRIVEN

The utility of MuG will be demonstrated through the development of **3 pilot projects** that will have early access to the MuG Virtual Research Environment services, providing valuable feedback and thus helping to develop the data management, computational infrastructure and analysis modules

1. Understanding the Chromatin reorganization during senescence
2. Multi-resolution dynamic map of Yeast chromatin
3. Physical properties of DNA and protein-DNA complexes

IMPACTS

MuG provides a virtual research environment addressed to the growing worldwide 3D/4D genomics community: general genomics, structural genomics, molecular modelling and medical genomics.

MuG will make an impact on **thousands of researchers** worldwide, ultimately contributing to the fast emerging field of personalized medicine.

The innovations developed by MuG will have a **strong impact on academia and industry alike.**

ACADEMIA AND RESEARCH INFRASTRUCTURES

Genomics and personalized medicine research community
Biosimulation and 3D Genomics community
HPC for Life Sciences initiatives
Users of European Infrastructures for HPC/Big Data
Genomics research community
Computer Science research community

LIFE SCIENCES INDUSTRY

Sequencing instrument vendors
Biotech/Pharma and Public Health

7 ANNEX II: Kick-off press release and media coverage

7.1 Press release text

Press Release **Wed., 9th December 2015**

Europe injects 3 million euros into three-dimensional genomics

- IRB Barcelona is to coordinate a *Horizon2020* bioinformatics project that seeks to lay the groundwork for the emerging field of 3D genomics.
- 3D genomics provides information about the structures adopted by folded DNA inside a cell and about how they change over time and in response to alterations in cell environment. Modesto Orozco, the coordinator of the project says, "The 3D perspective will allow us to better relate changes in the genome with the corresponding diseases, because although 1D information is relevant, it falls short."
- Over three years, the project aims to provide a set of methods and integrated databases that can be used to store and process the data deriving from studies devoted to 3D genomics.
- The European consortium comprises six international leading centres in method development and visualisation in 3D genomics.

Barcelona, 9 December 2015.- Today Barcelona sees the start of the European three-dimensional (3D) genomics project entitled "*Multi-scale complex genomics*". Coordinated by Dr. Modesto Orozco, at the Institute for Research in Biomedicine (IRB Barcelona), the project will be conducted over three years and has a budget of 3 million euros.

The goal is to standardise experiments in 3D genomics and the storage of data and to develop a set of protocols, methods, and processes by which to exploit these data, thus laying the groundwork for an emerging field that lacks organisation. "It is essentially a methodological project," explains Modesto Orozco. "The techniques used for 3D genomics are very new, they are not mature, and there are huge deficits in data processing. This makes the field unstable, above all with respect to the reproducibility of results," he adds.

Bringing science and technology closer

The project falls within "*e-Infrastructures for Virtual Research Environments*", part of the EU's *Horizon2020* Programme. The launch of this virtual collaboration initiative in genomics responds to the European Commission's roadmap to bring the scientific community closer to large research facilities, such as supercomputers. The idea is to progress over the next decade in a research field that is crucial for biomedicine, offering solutions for user needs and facilitating collaboration.

The project involves six European reference centres in programming, method development, and visualisation techniques for 3D genomics data. Labs at the following centres will be participating: IRB Barcelona; the Barcelona Supercomputing Center (BSC); the Institute of Human Genetics of the *Centre National de la Recherche Scientifique* (IGH-CNRS, France); The School of Pharmacy at the University of Nottingham (UK), the European Bioinformatics Institute (EMBL-EBI, UK) and the *Centre Nacional d'Anàlisi Genòmica-Centre for Genomic Regulation* (CNAG-CRG) that is located at the Barcelona Science Park, which is also home to IRB Barcelona.

From 1D to 3D

Genomics is one of the fields of biology developing most rapidly. In the last 15 years, the main challenge faced by biologists has been to obtain the sequences of the genome (one dimension) in order to predict how changes in DNA fragments are related with a particular disease. "The many 1D genomic studies in recent years have demonstrated that although the analysis of sequences provides valuable information, it is not sufficient to understand a given disease. The relationships remain obscure and probably are so because they depend on the 3D signal," explains the coordinator of the project.

The objective is now to move from the perspective of sequence, from letters, to understanding how chromatin, that is to say human DNA inside the cell, folds and how the structure of the fold can provide information about DNA function. "Also, we add a fourth dimension, which is seeing how chromatin structures change over time because of alterations in the external milieu or because of the functional needs of the cell," explains Orozco.

Through this project, Europe bolsters the high hopes expected from 3D and 4D genomics, fields producing many techniques that are developing rapidly. "All initiatives go through the stage of *forming*, *storming and performing*; in 3D genomics we are at the first stage and we are working towards keeping the storming stage to a minimum," says the coordinator.

As part of the technology package, the team plans to develop a viewer that allows users to move from the 1D observation of DNA, a format that biologists are familiar with, to offering folded structures, in which it is also possible to zoom in, going from a large scale to a smaller scale, both from the resolution point of view -from the metre to the angstrom (10^{-10} m)-, as well as that of time -from second to femtosecond (10^{-15} seconds)-.

"With the 3D vision of DNA, when we observe how the structure changes and adapts, I believe that we will start to find explanations for a lot of statistically relevant information deposited in data bases but that has escaped our understanding until now," says Orozco.

(This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 676556)

Image: 3D representation of a human DNA fragment (Copyright: Marc Martí-Renom, CNAG-CRG)

More information:

Sònia Armengou
Press Officer, IRB Barcelona
93 403 72 55/ +34 618 294 070

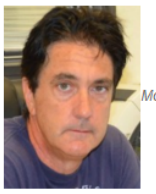
7.2 Coverage in specialized media

Some examples of the diffusion of the press release are shown below:

IT

Academics snag EU cash for 3-D genomics project

by *Nick Paul Taylor* | Dec 14, 2015 2:49am



Modesto Orozco

The European Union has coughed up €3 million ($3.3 million) for research into the 3-D structure of chromatin. Researchers will use the money to develop a set of protocols, methods and processes for the storage and analysis of data, laying the groundwork for an era in which understanding of the effects of nucleic acid sequences is supplemented by insights gleaned from the 3-D structures.

A team at the Institute for Research in Biomedicine in Barcelona, Spain, collected the money after persuading the organizers of the Horizon 2020 program of the need for investment in research into 3-D genomics. "The techniques used for 3-D genomics are very new, they are not mature and there are huge deficits in data processing. This makes the field unstable, above all with respect to the reproducibility of results," Modesto Orozco, the coordinator of the project, said in a statement. Orozco and his collaborators aim to use the €3 million to address these shortcomings.

The development of a viewer that enables researchers to see the 3-D structure of chromatin and zoom in on areas of interest is one objective. By showing researchers how chromatin folds and the effect this has on the function of the DNA, Orozco thinks the project can support breakthroughs. "The many 1D genomic studies in recent years have demonstrated that although the analysis of sequences provides valuable information, it is not sufficient to understand a given disease. The relationships remain obscure and probably are so because they depend on the 3-D signal," he said.

Orozco also wants to build in a fourth dimension, time, to show how the structure of the chromatin changes in response to external factors. To achieve these ambitions, the project has pulled together collaborators with a range of skills and capabilities. The Barcelona Supercomputing Center is on board to provide the computing horsepower, while the European Bioinformatics Institute is helping out with the handling of the biological data.

- read the release

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http://www.biocat.cat/en/news/europe-funds-3d-genomics-project-coordinated-irb-barcelona?language=en

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A piece of news

Europe funds 3D genomics project coordinated by IRB Barcelona

The study, being conducted by a consortium of six international institutions under the Horizon 2020 program, has received €3 millions

16.12.2015

Dr. Orozco is one of the top European researchers in simulating biological systems and a global benchmark in the study of macromolecular systems theory. - Photo: © IRB Barcelona.

A European 3D genomics project coordinated by Dr. Modesto Orozco, researcher at the Institute for Research in Biomedicine (IRB Barcelona), will receive €3 millions in funding under one of the actions of the European Union's Horizon 2020 program. The project is expected to last three years.

The study is being conducted by a consortium of six global leaders, which will work to standardize the way 3D genomics experiments are executed at large research facilities. Two other Catalan organizations, in addition to the IRB, are also participating: the Barcelona Supercomputing Center (BSC) and the National Center for Genomic Analysis-Center for Genomic Regulation (CNAG-CRG). The other participants are the Institute of Human Genetics of the French National Centre for Scientific Research, the University of Nottingham and the European Bioinformatics Institute.

Genomics is one of the fastest developing fields of biology. Previously, biologists had worked in the field of genomics to obtain the genome sequence (one dimension) and predict how changes in DNA fragments are connected to certain pathologies. Dr. Orozco warns that analyzing sequences is valuable but not enough to understand a specific disease.

Now the aim is to go from sequencing to understanding how chromatin –DNA condensed inside a cell– is folded into the space and how the folding structure can provide information on how DNA works. 3D genomics provides information about how DNA changes over time and in response to cell conditions. "With the 3D vision of DNA... I believe that we will start to find explanations for a lot of statistically relevant information deposited in databases but that has escaped our understanding until now," explains Orozco.

Modesto Orozco highlights that "It is essentially a methodological project," meaning the aim is to store data and create methodologies and processes to establish a network that can find meaning in all of the studies that are now underway and standardize experiments so they can be repeated. Orozco admits that the techniques are very new and not mature yet. "This makes the field unstable, above all with respect to the reproducibility of results," he adds.

Sources from the IRB Barcelona told Biocat that the consortium isn't a large association of partners; it has been created with the centers needed to make the project efficient. In fact, the consortium has a proven track record, as the teams have worked together before.

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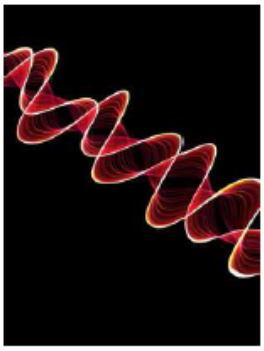
3D Genomics to the Rescue?

(January 22nd, 2016) **Mutations in one gene or many are behind numerous debilitating diseases. To be able to cure these diseases, we have to understand them. 3D genomics might do the trick, if it can overcome its teething troubles.**



Deoxyribonucleic acid, or DNA, has always fascinated scientists. Proof is the enormous research into its structure and function. Its alpha-helix nature, for instance, was confirmed by Rosalind Franklin in the 1950s, followed by the Robert Holley publication, in 1964, of the nucleic acid sequence of alanine transfer RNA. A bit later, Marshall Nirenberg and Philip Leder discovered that the genetic code is read in triplets.

One of the most important developments, however, came from British biochemist, Frederick Sanger. In 1975, he published a paper (together with lab tech Alan Coulson), introducing a new method of sequencing DNA. His method, today simply called Sanger sequencing, has since revolutionised genetics. Although the technique was a breakthrough in genetics, it cannot be used to study, for instance, DNA function. This is where 3D genomics comes in, which provides powerful experimental approaches to predict and study DNA's role when coupled to endogenous protein or environmental factors.

In contrast to Sanger sequencing and its variations, which analyses the primary sequence of DNA to search for individual nucleotide changes that might affect, for instance, disease development, 3D genomics looks at the more complex secondary and tertiary structures of DNA. Techniques, such as Chromosome Conformation Capture (3C) and its derivatives, DNA adenine methyltransferase identification (DamID) and Chromatin interaction analysis (ChIA) reveal intramolecular interactions between DNA and proteins. Employing these techniques has helped elucidate the molecular basis of, for instance, cancer or Duchenne muscular dystrophy.

As helpful as these methods are to understand complex diseases, they also create large amounts of data that need to be interpreted correctly. In December, the new project "Multi-Scale Complex Genomics" or MuG started, aiming to improve and standardise 3D genomics to make it available for a wider scientific audience. Funded by the European Commission, which promised to provide three million euros to five research centres in Spain, the United Kingdom and France, MuG wants to address some of the biggest problems that bug the field. These include the huge background noise in 3D genomics data, non-standardised analysis methods and miscommunication between bioinformatics databases.

"We are trying to correlate the genome with the phenome using only one dimension, while functionality of DNA depends on genome organisation in the space. What we are doing now will be like organising air traffic using only one dimension instead of three. A chaos, isn't it?" explains Modesto Orozco, coordinator of MuG project at the Institute for Research in Biomedicine (IRB) Barcelona. "This project will help nucleate and organise the community, fuelling the integration between high performance computing and genomics and moving towards a more realistic view of the genome organisation," he

http://www.medicineonline.es/es/noticias/europa-impulsa-con-3-millones/25282/

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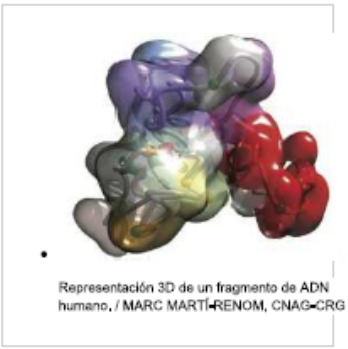
Europa impulsa con 3 millones de euros la genómica tridimensional

JANO.es · 10 diciembre 2015 13:09

El IRB Barcelona coordina un proyecto cuyo objetivo es estandarizar la manera de ejecutar experimentos en este campo, almacenar los datos y explotarlos a través de la creación de un paquete de protocolos.



Representación 3D de un fragmento de ADN humano. / MARC MARTÍ-RENOM, CNAG-CRG

El Dr. Modesto Orozco, del Instituto de Investigación Biomédica (IRB Barcelona), coordina desde ayer el proyecto europeo en genómica tridimensional (3D) 'Multi-scale complex genomics', cuya duración prevista son 3 años, y que ha recibido una financiación de 3 millones de euros de la UE.

El objetivo es estandarizar la manera de ejecutar experimentos en genómica 3D, almacenar los datos y explotarlos a través de la creación de un paquete de protocolos, metodologías y procesos que ordenen un campo emergente falto de esta infraestructura. "Es un proyecto esencialmente metodológico", explica Orozco, "Las técnicas para hacer genómica 3D son muy nuevas, no están maduras y hay mucha carencia en el procesado de los datos, lo que produce una sensación de fragilidad, sobre todo por la poca reproducibilidad de los resultados", añade.

El proyecto se enmarca en de las acciones 'e-Infraestructures for Virtual Research Environments', del programa Horizon2020 de la Unión Europea. La creación de este entorno de colaboración virtual en genómica responde a la hoja de ruta de la Comisión Europea para acercar la comunidad científica a las grandes infraestructuras de investigación, tales como los supercomputadores. La visión de futuro es acelerar la investigación en un campo clave para la biomedicina de la próxima década, ofreciendo soluciones que responden a las necesidades de los usuarios y facilitan la colaboración.

El proyecto implica seis instituciones de referencia en Europa en programación, desarrollo de métodos y técnicas de visualización de datos genómicos 3D. Lo componen laboratorios del IRB Barcelona, el Barcelona SuperComputing Center (BSC), el Institute of Human Genetics del Centre National de la Recherche Scientifique (IGH-CNRS), la University of Nottingham, el European Bioinformatics Institute (EMBL-EBI) y el Centro Nacional de Análisis Genómico-Centro de Regulación Genómica (CNAG-CRG), infraestructura ubicada en el Parque Científico de Barcelona, donde también está localizado el IRB Barcelona.

De una dimensión a tres

La genómica es uno de los campos de la biología que está evolucionando más rápidamente. En los últimos 15 años el reto principal de los biólogos ha sido obtener las secuencias del genoma (una dimensión) para predecir cómo los cambios en fragmentos del ADN se relacionaban con una determinada patología. "La gran cantidad de estudios en genómica 1D de estos últimos años han demostrado que el análisis de las secuencias, aunque nos aportan información valiosa, no es suficiente para entender una determinada patología. Las conexiones quedan enmascaradas y probablemente sea porque dependen de la señal 3D", explica el coordinador del proyecto.

Ahora el objetivo es pasar de esta visión de secuencia, de letras, a entender cómo la cromatina, es decir el ADN humano dentro de la célula, está replegado en el espacio y cómo la estructura del

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7.3 Coverage in general media

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Colaboración virtual y genómica tridimensional española

BY JUAN ROYO ABENIA ON 9 DICIEMBRE, 2015 RSC

El Instituto de Investigación Biomédica (IRB) de Barcelona coordina un proyecto *Horizon2020* en bioinformática para poner orden la genómica 3D. Este campo emergente ofrece información de la estructura que adopta el ADN replegado dentro de la célula, como varía en el tiempo y por respuesta a condiciones celulares. Se pretende en 3 años ofrecer un paquete de métodos y bases de datos integradas para guardar y procesar los estudios en genómica 3D.

Ha comenzado en Barcelona el proyecto europeo en genómica tridimensional (3D) *"Multi-scale complex genomics"*, con una duración de 3 años y con una financiación de 3 millones de euros, coordinado por el Dr. Modesto Orozco, del IRB.

El objetivo es estandarizar la manera de ejecutar experimentos en genómica 3D, almacenar los datos y explotarlos a través de la creación de un paquete de protocolos, metodologías y procesos que ordenen un campo emergente falto de esta infraestructura.

> *Es un proyecto esencialmente metodológico. Las técnicas para hacer genómica 3D son muy nuevas, no están maduras y hay mucha carencia en el procesado de los datos, lo que produce una sensación de fragilidad, sobre todo por la poca reproducibilidad de los resultados* **Modesto Orozco**

Acercar la ciencia y la tecnología

El proyecto se enmarca dentro de las acciones *"e-Infraestructures for Virtual Research Environments"*, del programa *Horizon2020* de la Unión Europea. La creación de este entorno de colaboración virtual en genómica responde a la hoja de ruta de la Comisión Europea para acercar la comunidad científica a las grandes infraestructuras de investigación, tales como los supercomputadores. La visión de futuro es acelerar la investigación en un campo clave para la biomedicina de la próxima década, ofreciendo soluciones que responden a las necesidades de los usuarios y facilitan la colaboración.

El proyecto implica seis instituciones de referencia en Europa en programación, desarrollo de métodos y técnicas de visualización de datos genómicos 3D. Lo componen laboratorios del IRB Barcelona, el Barcelona SuperComputing Center (BSC), el *Institute of Human Genetics* del *Centre National de la Recherche Scientifique*

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http://www.lavanguardia.com/vida/20151209/30694707508/el-irb-recibe-el-encargo-europeo-para-estructurar-la-genomica-tridimensional.html

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El IRB recibe el encargo europeo para estructurar la genómica tridimensional

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Barcelona, 9 dic (EFE).- El Instituto de Investigación Biomédica (IRB) de Barcelona ha recibido el encargo de coordinar el proyecto europeo Horizon2020 en bioinformática, dotado con tres millones de euros, para poner orden en el campo emergente de la genómica tridimensional.

El proyecto "Multi-scale complejo genomics" se ha puesto en marcha hoy en Barcelona, con una duración de tres años, y coordinado por el doctor Modesto Orozco, quien ha explicado que el objetivo es estandarizar la manera de ejecutar experimentos en genómica 3D, almacenar los datos y explotarlos a través de la creación de un paquete de protocolos, metodologías y procesos que ordenen un campo emergente falto de esta infraestructura.

"Es un proyecto esencialmente metodológico -ha añadido Orozco- ya que las técnicas para hacer genómica 3D son muy nuevas, no están maduras y hay mucha carencia en el procesado de los datos, lo que produce una sensación de fragilidad, sobre todo por la poca reproducibilidad de los resultados"

El proyecto se enmarca dentro de las acciones "e-Infraestructuras for Virtual Research Environments", del programa Horizon2020 de la Unión Europea.

La creación de este entorno de colaboración virtual en genómica responde a la hoja de ruta de la Comisión Europea para acercar la comunidad científica a las grandes infraestructuras de investigación, como el uso de

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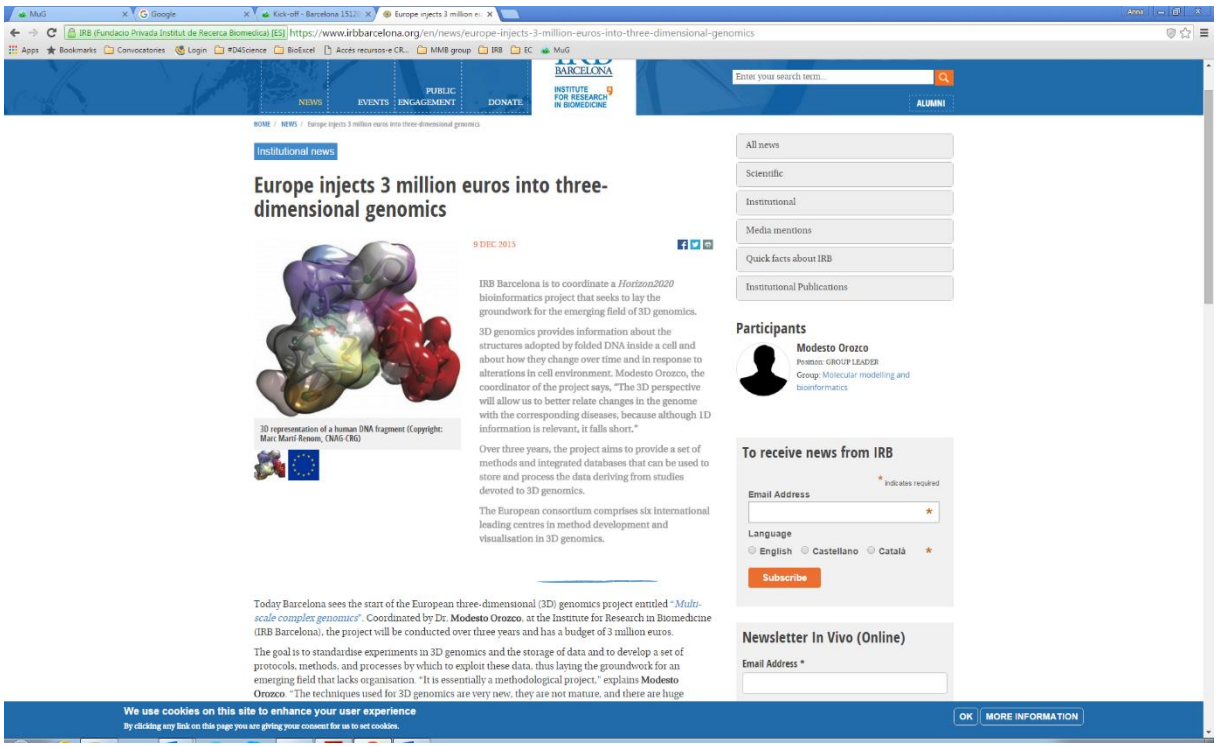
7.4 Coverage in partners websites

MuG partners' institutions echoed the press release in their respective websites:

IRB Barcelona



CNAG-CRG

Bringing order to the emerging field of 3D-Genomics

The project falls within **"e-Infrastructures for Virtual Research Environments"**, part of the EU's Horizon2020 Programme (https://ec.europa.eu/programmes/horizon2020/) and involves six European reference centres in programming, method development, and visualisation techniques for 3D genomics data. Labs at the following centres will be participating: IRB Barcelona (http://www.irbbarcelona.org/es); the Barcelona SuperComputing Center (BSC) (https://www.bsc.es/); the Institute of Human Genetics of the Centre National de la Recherche Scientifique (IGH-CNRS) (http://www.igh.cnrs.fr/EN/); the University of Nottingham (https://www.nottingham.ac.uk/); the European Molecular Biology Laboratory (EMBL-EBI) (http://www.ebi.ac.uk); and the Centre Nacional d'Anàlisi Genòmica (CNAG-CRG).

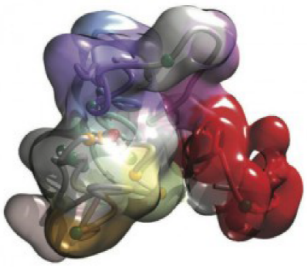
The role of the CNAG-CRG in the project

The CNAG-CRG acts as coordinator of WP3 for Multi-scale visualization of genomics data. We are in charge of providing a visualizer of genomics data in 3D and 4D (in time). The Structural Genomics Team at the CNAG-CRG will deploy its TADkit software (http://www.3DGenomes.org) as a platform for visualizing the genomics data and simulation provided by the other partners in the MuG consortium.

From 1D to 3D

3D genomics provides information about the structures adopted by folded DNA inside a cell and about how they change over time and in response to alterations in cell environment. Modesto Orozco, the coordinator of the project says, "The 3D perspective will allow us to better relate changes in the genome with the corresponding diseases, because although 1D information is relevant, it falls short."

More information:



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BSC

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

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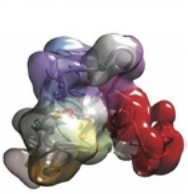
Europe injects 3 million euros into three-dimensional genomics

BSC

9 Dec 2015



IRB Barcelona is to coordinate a *Horizon2020* bioinformatics project that seeks to lay the groundwork for the emerging field of 3D genomics.

3D genomics provides information about the structures adopted by folded DNA inside a cell and about how they change over time and in response to alterations in cell environment. Modesto Orozco, the coordinator of the project says, "The 3D perspective will allow us to better relate changes in the genome with the corresponding diseases, because although 1D information is relevant, it falls short."

Over three years, the project aims to provide a set of methods and integrated databases that can be used to store and process the data deriving from studies devoted to 3D genomics.

The European consortium comprises six international leading centres in method development and visualisation in 3D genomics.

Today Barcelona sees the start of the European three-dimensional (3D) genomics project entitled *"Multi-scale complex genomics"*. Coordinated by Dr. **Modesto Orozco**, at the Institute for Research in Biomedicine (IRB Barcelona), the project will be conducted over three years and has a budget of 3 million euros.

The goal is to standardise experiments in 3D genomics and the storage of data and to develop a set of protocols, methods, and processes by which to exploit these data, thus laying the groundwork for an emerging field that lacks organisation. "It is essentially a methodological project," explains **Modesto Orozco**. "The techniques used for 3D genomics are very new, they are not mature, and there are huge deficits in data processing. This makes the field unstable, above all with respect to the reproducibility of results," he adds.

Bringing science and technology closer

The project falls within *"e-Infrastructures for Virtual Research Environments"*, part of the EU's *Horizon2020* Programme. The launch of this virtual collaboration initiative in genomics responds to the European Commission's roadmap to bring the scientific community closer to large research facilities, such as supercomputers. The idea is to progress over the next decade in a research field that is crucial for biomedicine, offering solutions for user needs and facilitating collaboration.

The project involves six European leading centres in programming, method development, and visualisation techniques for 3D

8 ANNEX III: JOINT DISSEMINATION OF EUROPEAN E-INFRA PROJECTS

MuG was represented in the poster presented by e-Infra EU in the RDA 7th plenary session in Tokyo, Japan (March 1st to 3rd, 2016).