

# Multiscale Complex Genomics



Project Acronym: MuG Project title: Multi-Scale Complex Genomics (MuG) Call: H2020-EINFRA-2015-1 Topic: EINFRA-9-2015 Project Number: 676556 Project Coordinator: Institute for Research in Biomedicine (IRB Barcelona) Project start date: 1/11/2015 Duration: 36 months

# Deliverable 2.8: Report on the MuG training programme

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

Due date: 31/10/2018 Actual submission date: 09/11/2018

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

# Document history

Version	Contributor(s)	Partner	Date	Comments
0.1	Anna Montras	IRB Barcelona	10/09/2018	First draft
0.2	Mark McDowall	EMBL-EBI	11/10/2018	Inputs section 4 (developer training)
0.3	Anna Montras	IRB Barcelona	05/11/2018	Second draft
0.4	Andrew Yates	EMBL-EBI	08/11/2018	Revision
0.5	Javier Conejero	BSC	09/11/2018	Additions to section 2
1.0			09/11/2018	Approved by Supervisory Board



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# **Executive summary**

Training represents a key tool to engage end users in the use of the MuG VRE, and thus training efforts undertaken during the first reporting period (November 2015-April 2017) were reported in D2.4. The present report will thus focus on training activities carried out during the second reporting period, while still providing a complete list of all training activities carried out during the 3 years of duration of the project for easy reference. Among the achievements of the last year and a half, we would like to highlight the enhancement of the hands-on contents of all training courses, which is the most valued aspect of MuG training.by participants. In addition, the basis for developer-oriented training has also been established with a first pilot training course on the use of the MuG tool-wrapping API. Overall, **>250** people have participated in training events in which MuG has been featured, **110** of them in actual practical training on the use of the MuG VRE.



# **1 INTRODUCTION**

This report builds up on the training plan developed at the beginning of the project (D2.3) and whose preliminary implementation results were reported in D2.4.

Different levels of training activities have been successfully implemented. During the first year, training focused in individual tools, making our potential user community aware of the benefits to be offered by the MuG VRE, such as ease of use thanks to the integrated tools and customized workflows<sup>1</sup>.

By M18 and more notably following the release of the first version of the MuG VRE (November 2017), the focus moved to showcasing the multi-scale concept of the VRE through real biological use cases. This kind of workshops target end-users of the MuGVRE, who are either familiar with tools and want to find out the benefits of the VRE, or who simply would value using the VRE in first instance as the means of getting familiar with such analysis tools.

During the last year of the project training activities targeting end-users and involving all partners were intensified. In addition, in September 2018 a pilot training workshop was organized aimed at tool developers interested in integrating their own tools into the MuG VRE.

Joint activities and promotion of events with other EU e-infrastructures have helped in the implementation of the MuG training plan and will become key towards securing the sustainability of such services beyond the end of the MuG 3-year grant. As an example of such collaboration with EU initiatives we would like to highlight the co-organization of workshops and webinars with BioExcel, with which a Memorandum of Understanding has been signed, and the advertising of MuG training activities through the ELIXIR Europe training portal.

# 2 MuG TRAINING PLAN

The MuG training strategy was outlined in D2.4 and its implementation has successfully concluded during the second reporting period. The MuG strategy is based on the following main points:

- 1. Courses are tailored to **different kinds of audiences** according to their need of interaction with the VRE.
- 2. To maximize the impact, MuG training events are **co-located with key gatherings** of the scientific community, organized in strategic locations that foster the participation of the target audiences:
  - The first MuG workshop aimed at beta-users (April 2017) and the MuG tool API workshop aimed at tool developers (September 2018) conveniently took place at the facilities of EMBL-EBI.
  - A MuG demo workshop to present the first MuG VRE public release was colocated with the Barcelona BioMed conference on Multidimensional Genomics, co-organized by 3 MuG PIs.

<sup>&</sup>lt;sup>1</sup> Deliverable 2.4: Monitoring of the plan for the dissemination and use of knowledge.



- A joint workshop with BioExcel CoE on multi-resolution nucleic acids simulation was conveniently co-located and co-organized with the ISQBP2018, the meeting of the International Society of Quantum Biology and Pharmacology<sup>2</sup>
- 2. **Cross-collaboration with relevant initiatives** has been established: joint training activities with partner initiatives or relevant institutions have been promoted as an important platform to drive the use of the MuG innovations:
  - BioExcel CoE: a Memorandum of Understanding for collaboration between MuG and BioExcel establishes training as one of the key activities were both initiatives have clear synergies. The collaboration with BioExcel CoE is regarded as strategic to grant sustainability of MuG training activities. Collaborations have included featuring MuG in several webinars on the use of biosimulation tools that are integrated in the VRE and a joint MuG-BioExcel hands-on course on multi-resolution nucleic acids simulations, using both MuG and BioExcel developments.
  - The PRACE course organized from BSC on molecular simulations is regarded as an important platform to spread our technologies and databases in the entire bio-simulation community.
  - Hands-on training on the MuGVRE has been integrated in the 3DAROC course organized by the Gulbenkian Training Programme in Bioinformatics together with the developers of TADbit/TADkit 3D chromatin analysis and visualization tools.
- Beyond MuG's own media resources (website, social media, partner institutional websites) MuG has received the support from partner initiatives, associations or institutions, including <u>Epigenesys</u> (https://www.epigenesys.eu/), <u>Bioinformatics</u> <u>Barcelona</u> (<u>http://www.bioinformaticsbarcelona.eu/</u>), <u>Barcelona Institute of Science and Technology</u> (<u>https://bist.eu/</u>), <u>EMBL-EBI's training portal</u> (<u>https://www.ebi.ac.uk/training</u>) see annex 8.5
- Issued training materials for end users (workshops) are made available on the website for the benefit of a wider audience (http://www.multiscalegenomics.eu/MuGVRE/training/)

A full list of training activities in which MuG has taken part is provided in Table 1:

**Table 1**: List of completed training events (blue shadowed rows correspond to courses fully organized byMuG)

DATE	Title	LOCATION	Participant	Organizer	Type training	Audience size
04/02/2016	PATC Course: Programming Distributed Computing Platforms with COMPSs	Barcelona, Spain	BSC	PRACE, BSC	Technology used in MuG development	25
10-	3DAROC16: 3C-based	Oeiras,	IRB, CNAG-	GTPB, CNAG-	MuG	14
14/10/2016	data analysis and 3D	Portugal	CRG	CRG, <b>MuG</b>	integrated	

<sup>&</sup>lt;sup>2</sup>https://bioexcel.eu/isqbp-presidents-meeting-mug-bioexcel-multi-resolution-nucleic-acids-simulations-workshop-in-barcelona/



	reconstruction of chromatin folding				tools + MuG VRE	
14/03/2016	PATC Course. Simulation Environments for Life Sciences	Barcelona, Spain	IRB, BSC	PRACE, BSC	Tools integrated in MuG	26
27/09/2016	<u>Workshop: Design</u> <u>your e-infrastructure</u>	Krakow, Poland	IRB, BSC	EGI.GEANT,E UDAT, OpenAIRE	Sustainability of e- infrastructures	15
02/02/2017	PATC: Programming Distributed Computing Platforms with COMPSs	Barcelona, Spain	BSC	PRACE, BSC	Technology used in MuG development	28
14/03/2017	PATC Course. Simulation Environments for Life Sciences	Barcelona, Spain	IRB, BSC	PRACE, BSC	Tools integrated in MuG	30
3-7/04/2017	Chromosomal conformation	Barcelona, Spain	CNAG-CRG	CNAG-CRG	Tools integrated in MuG	16
10- 11/04/2017	Multi-scale study of 3D Chromatin structure	Hinxton, UK	All	<b>MuG</b> , EMBL- EBI	Hands-on course on MuG VRE	18
14- 17/05/2017	Tutorial at CCGRID2017: Programming distributed platforms with PyCOMPSs	Madrid, Spain	BSC	ARCOS/UC3 M, IEEE	Technology used in MuG development	10
28/08- 1/09/2017	Tutorial at EURO-PAR 2017 – 23 <sup>rd</sup> Internaltional European Conference on Parallel and distributed computing	Santiago de Compostel a, Spain	BSC	Univ. Santiago de Compostela, CiTIUS	Technology used in MuG development	10
9/07/2017	Tutorial at ACACES 2017 – 13 <sup>th</sup> International Summer School on Advanced Computer Architecture and Compilation for High-Performance and Embedded systems	Fiuggi, Italy	BSC	HiPEAC Network of Excellence	Technology used in MuG development	40-60
13/07/2017	PyCOMPSs Tutorial at EuroPython 2017	Rimini, Italy	BSC	EuroPython Society	Technology used in MuG development	30
20/07/2017	NAFlex, a web server for the study of nucleic acid flexibility	(online)	IRB	BioExcel CoE	Webinar on tools integrated in MuG	~20
15/11/2017	Multi-scale study of 3D Chromatin structure (co-localized with Barcelona BioMed conference)	Barcelona, Spain	IRB, BSC, CNAG	MuG, IRB	Demo course on MuG VRE	35



8/03/2018	Task-Based Parallel Programming with PyCOMPSs at SIAM Conference on Parallel Processing for Scientific Computing (PP18)	Tokyo, Japan	BSC	Society for Industrial and Applied Mathematics	Technology used in MuG development	20
11/04/2018	BioExcel Webinar Series – MC-DNA: A web server for the detailed study of the structure and dynamics of DNA and chromatin fibers.	(online)	IRB	BioExcel CoE	Webinar on tools integrated in MuG	~20
13-14/12/ 2017	Multi-scale study of 3D chromatin structure. 2 <sup>nd</sup> edition	Barcelona, Spain	IRB, BSC	MuG	Hands-on course on MuG VRE	11
2-4/05/2018	CECAM workshop: Epigenetics and Multiscale Genomics	Lausanne, Switzerland	IRB	CECAM, EPFL	Theorectical workshop	28
22/06/2018	Multi-resolution Nucleic Acids Simulations. A joint MuG-BioExcel workshop	Barcelona, Spain	IRB, BSC	BioExcel CoE, MuG	Hands-on course on MuG VRE	18
17- 21/09/2018	3DAROC18:3C-based analysis and 3D- reconstruction of chromatin folding.	Oeiras, Portugal	CNAG-CRG	GTPB, CNAG- CRG	Hands-on MuG integrated tools + MuG VRE	14

# **3 END-USER TRAINING**

Following the recommendations offered by MuG advisors and reviewers, training activities were structured around real biological use-cases that were developed through close collaboration between developers and pilot projects. Given the essential role of training in engaging the end-user community in the testing of the VRE, the number of workshops carried out during the second period was intensified and those were strategically planned to take place around relevant milestones of the project (VRE public release, etc.) or to be co-located with large community gatherings that counted with the presence of leaders in the field.

# 3.1 Multi-scale simulation of 3D chromatin structure (Demo)

In November 2017, MuG PIs Modesto Orozco (coordinator), Marc A. Martí-Renom and Giacomo Cavalli, co-organized the conference *Multidimensional Genomics: the 3D/4D organization of chromatin*. This represented a unique opportunity for MuG to co-locate the presentation of the first public release of the VRE with a large gathering of the 3D/4D genomics community. To maximize the impact and reach the largest possible audience, a demo format workshop was organized and dissemination and communication efforts were intensified, with the release of the MuG video and a press-release that had an ample impact in different kinds of media.

The demo workshop took place at the Institut d'Estudis Catalans, in Barcelona, Spain.





DATE	Title	LOCATION	Participant	Organizer	Type training	Audience size
15/11/2017	Multi-scale study of 3D Chromatin structure (co-localized with Barcelona BioMed conference)	Barcelona, Spain	IRB, BSC, CNAG	MuG, IRB	Demo course on MuG VRE	35

# 3.1.1. Course description

A full description of the course, together with the generated training materials, is available on the MuG website: <u>http://www.multiscalegenomics.eu/MuG/multi-scale-study-3d-chromatin-structure-2/</u>:

## Course overview

The workshop introduced delegates to the Virtual Research Environment (VRE), created by the Multi-scale complex Genomics project (MuG), to facilitate the analysis and interpretation of the 3D and 4D structure genome.

The MuG VRE integrates a range of data from genome annotation to 3D folding and DNA flexibility. Recent studies have shown the role that genome organisation can play in gene expression and the VRE has been designed to provide a way of analysing such data.

The workshop will demonstrate how to use the multi-scale features of the VRE through integrated tools for the study of Nucleosome dynamics and for the analysis of Hi-C data and visualization of 3D models.

#### Audience

Aimed at both experimental (bench-based) researchers and bioinformaticians; additionally it may be of interest to tool developers who wish to integrate their tools into the VRE.

Participants should have knowledge of genome organisation and the role it can play within the nucleus.

## Syllabus, tools and resources

During this workshop participants learn about:

- The MuG Virtual Research Environment (VRE) initiative for 3D genomics
- Nucleosome architecture. NucleR and Nucleosome Dynamics
- Global chromatin structure from Hi-C, interaction matrices and TADs (topologically associating domains)



## <u>Programme</u>

Time	Торіс	Speakers
14:30-15:00	MuG VRE presentation	Josep Lluis Gelpí (BSC)
15:00-16:00	TADbit and TADkit: Generation of Hi-C interaction matrices from Hi-C data and visualization of 3D models	David Castillo (CNAG-CRG)
16:00-16:30	Coffee break	
16:30-17:30	Nucleosome Dynamics	Ricard Illa (IRB Barcelona) Jürgen Walther (IRB Barcelona)
17:30-18:30	Conclusions and feedback	

## 3.1.2. Feedback and conclusions

The course was originally conceived as a hands-on workshop limited to 25 people. However, the event was largely overbooked and, since the public release of the VRE was to take place on the same dates, it was eventually decided to open it to a larger number of people. For those interested in a practical course, a hands-on workshop was offered a month later also in Barcelona (see section 3.2).

As a general conclusion, the demo workshop was a great opportunity to make the community aware of the release of the MuG VRE and all the advantages it could bring. However, participants' feedback reflected that actual details on the use of the VRE were best assimilated with a more reduced number of people.





The results of the training survey should a quite heterogeneous profile of the participants, ranging from masters students (8%) to senior academics (15%) and with 38% and 31% of postdocs and PhD students respectively. However, only ~50% of participants answered the survey.

Although the overall rating of the course was slightly hindered by the quality of the projections and the demo format, overall, all sessions obtained above 60% positive feedback and 77% intend to use the MuG VRE tools in their future work. The integrated workflows and data management offered by the





VRE is the MuG aspect that participants value the most (85%) and 46% also appreciate the function of the website as a source for community related news and the offer of training services.

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# 3.2 Multi-scale study of 3D chromatin structure: 2<sup>nd</sup> edition

4 A full description of the course, together with the generated training materials, is available on the MuG website: <u>http://www.multiscalegenomics.eu/MuG/multi-scale-study-3d-</u> <u>chromatin-structure-2nd-edition/</u>



Multi-scale Genomics workshop Multi-scale study of 3D chromatin structure: 2<sup>nd</sup> Edition



DATE	Title	LOCATION	Participant	Organizer	Type training	Audience size
13-14/12/ 2017	Multi-scale study of 3D chromatin structure. 2 <sup>nd</sup> edition	Barcelona, Spain	IRB, BSC	MuG	Hands-on course on MuG VRE	11

# 3.2.1. Course description

Course overview

This workshop will introduce delegates to a Virtual Research Environment (VRE), created by the Multi-scale complex Genomics project (MuG), to facilitate the analysis and interpretation of the 3D and 4D structure of the genome.



The MuG VRE integrates a range of data from genome annotation to 3D folding and DNA flexibility. Recent studies have shown the role that genome organisation can play in gene expression and the VRE has been designed to provide a way of analysing such data. The course will explore how to use the multi-scale features and integrated tools of the MuG VRE through the study of real biological examples

## <u>Audience</u>

The workshop is aimed at both experimental (bench-based) researchers and bioinformaticians; additionally it may be of interest to tool developers who wish to integrate their tools into the VRE.

Participants should have a Master's degree or higher understanding of biology and have knowledge of genome organisation and the role it can play within the nucleus.

## Syllabus, tools and resources

During this workshop participants will learn about:

- The Multi-scale complex Genomics project (MuG)
- The MuG Virtual Research Environment (VRE)
- Nucleosome dynamics
- Hi-C, interaction matrices and TADs (topologically associating domains)
- Protein-DNA interactions

## <u>Outcomes</u>

After the workshop, participants will be able to:

- Navigate the MuG VRE
- Model and analyse a protein-DNA complex at the atomistic scale
- Process Hi-C data sets to produce interaction matrices and TADs
- Apply the MuG VRE to participants own data sets.

## 3.2.2. Programme

Time	Торіс	Instructor
Day 1 (Wedne		
9:00 – 9:30	Registration and welcome	
9:30 – 10:00	MuG and participants introduction	Modesto Orozco
10:00 – 10:30	MuG VRE workspace presentation	
10:30 – 11:30	Presentation of Nucleosome Dynamics	Ricard Illa /Federica Battistini
11:30 – 12:00	Coffee Break	
12:00 - 13:30	Use case (application of Nucleosome Dynamics)	Ricard Illa / Federica Battistini
13:30 - 14:30	Lunch	
14:30 – 16:00	Coarse grained model of DNA. Build and analyze a sequence of interest.	Jürgen Walther
16:00 - 16:30	Coffee Break	
16:30 – 17:30	Coarse grained model of chromatin; Generation and analysis of chromatin fiber structures.	Jürgen Walther
17:30 – 18:00	Day 1 wrap-up , open questions and answers	



Day 2 (Thursday 14th December)								
9:00 – 10:45	Presentation of Protein-DNA and protein-protein docking tools	Brian Jiménez						
10:45 – 11:15	Coffee break							
11:15 – 13:00	Protein-DNA interactions, DNA flexibility and binding specificity.	Charles Laughton						
13:00 - 14:00	Lunch							
14:00 - 15:30	Presentation of TADbit: generation of Hi-C interaction matrices from Hi-C data	David Castillo						
15:30 – 16:00	Coffee break							
16:00 – 17:30	Generation of populations of structures that satisfy the Hi-C interaction matrices. Visualization of 3D models using TADkit	David Castillo						
17:30 – 18:00	Course wrap up and feedback							

## 3.2.3. Feedback

The satisfaction survey was answered by 81% of participants, which were in their majority (80%) PhD students. 88% of participants rated the course as good or satisfactory.

Overall, 89% found the balance between theoretical and practical contents correct and all participants that filled in the survey either intend to use the VRE (67%) or will consider it (33%). 100% of participants would recommend the course. What is you overall rating for the content and delivery of the course? 9 responses



The course was a good source of feedback for VRE developers on how

to improve the functionality and user experience, and also with regards to the demands of the end users in terms of tool offer. The raw answers are available in Annex II.







# **3.3.** Multi-resolution Nucleic Acids Simulations. A joint MuG-BioExcel workshop.



Multi-resolution Nucleic Acids Simulations. A joint MuG-BioExcel workshop.

DATE	Title	LOCATION	Participant	Organizer	Type training	Audience size
22/06/2018	Multi-resolution Nucleic Acids Simulations. A joint MuG-BioExcel workshop	Barcelona, Spain	IRB, BSC	BioExcel CoE, MuG	Hands-on course on MuG VRE	18

This workshop not only represents the collaboration and the synergies between two complementary e-infrastructures such as BioExcel CoE and MuG VRE, but it also takes advantage of the co-location with a key scientific gathering (ISQBP President's meeting 2018) to maximize the impact. The workshop trained participants in the use of the infrastructures and services provided by both projects.

# 3.3.1. Course description

## Course overview

**Nucleic acids** (NAs) are biomolecules essential to all known forms of life that exhibit a remarkable structural and functional diversity. NAs are studied through several different techniques, including experimental and theoretical methods. The notorious improvements of the latter, together with the increased computation power, explain their widespread use in improving our understanding of their structure and function. Giving the **multiscale nature of** 



NAs, different theoretical disciplines like quantum chemistry, molecular mechanics and mesoscopic biophysical approaches are considered.

Multiscale Complex Genomics (MuG) project was conceived to tackle the latest computational challenges on the **multiscale nature of NAs**, connecting this community to the **HPC** and **Big Data** world and providing a suitable set of **tools** and **infrastructure** to integrate the navigation in genomics data from sequence (1D) to 3D/4D chromatin dynamics.

BioExcel Center of Excellence is as a **central hub for biomolecular modelling and simulations**, with a mission to enable scientists to fully exploit the power of data and computing e-infrastructure by providing support to non-experts and advanced users.

The purpose of this workshop is to:

- Discover the set of **multiscale genomics modelling and simulation tools** used in the MuG project.
- Learn how to easily run them through the BioExcel Cloud Portal infrastructure.
- Have a first contact with the MuG Virtual Research Environment (**VRE**), a GUI integrating the set of tools with an interactive and graphical interface.

#### Audience

The workshop is aimed at both experimental researchers and bioinformaticians; additionally it may be of interest to tool developers who wish to integrate their tools into the MuG VRE.

No software installation will be necessary, Virtual Machines (VMs) will be deployed on-line through the BioExcel Cloud Portal. The room is equipped with computers.

#### <u>Outcomes</u>

After this course you should be able to:

- Prepare and simulate NAs mesoscopic and atomistic models, both in a High-Throughput way (workflows, command-line executions) as well as using a user-friendly GUI interface.
- Obtain flexibility parameters out of the NAs simulations: PCA, Helical Parameters, Distance Contact Maps, NMR observables, etc.

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Friday 22 J	Friday 22 June 2018						
Start	End	Title (Presenter name)					
09:00	10:00	Welcome & Introduction: BioExcel & MuG ( <b>Modesto Orozco, MuG project coordinator</b> – IRB Barcelona, <b>Josep Lluís Gelpí</b> , BSC; <b>Adam Hospital</b> , IRB Barcelona)					
10:00	11:00	Mesoscopic Models ( <b>Jürgen Walther</b> , IRB Barcelona)					



11:00	11:30	Coffee Break
11:30	12:30	MD Atomistic Models ( <b>Pau Andrio</b> , BSC Barcelona)
12:30	13:30	Ensemble/Trajectory Analysis ( <b>Adam Hospital</b> , IRB Barcelona)
13:30	15:00	Lunch / MareNostrum IV Supercomputer Visit
15:00	15:30	Multi-resolution Nucleic Acids Simulations Integration VRE Chromatin Dynamics (ChromDyn) ( <b>Jürgen Walther</b> , IRB Barcelona)
15:30	16:00	Multi-resolution Nucleic Acids Simulations Integration VRE MonteCarlo DNA (MCDNA) ( <b>Jürgen Walther</b> , IRB Barcelona)
16:00	16:30	Multi-resolution Nucleic Acids Simulations Integration VRE Python Molecular Dynamics library (PyMD) ( <b>Pau Andrio</b> , BSC Barcelona)
16:30	17:00	Multi-resolution Nucleic Acids Simulations Integration VRE Nucleic Acids Flexibility (NAFlex) ( <b>Adam Hospital</b> , IRB Barcelona)
17:00	18:00	Q & A + Wrap Up Session ( <b>All speakers</b> )





# 3.4. 3DAROC18: 3C-based data analysis and 3D reconstruction of chromatin folding

3DAROC is organized every two years by the Gulbenkian training Programme in Bioinformatics of the Instituto Gulbenkian de Ciência (Portugal) and the team of Marc A. Martí-Renom at CNAG-CRG (developers of TADbit 3C-data analysis software and TADkit 3D genome visualizer). In the 2016 edition of the course multiscale aspects of 3D genome study were incorporated into the course programme, with an additional day including sessions on atomistic simulation tools and presenting the MuG VRE concept to participants with very good acceptance. Following the public release of the MuG VRE, the 2018 edition of 3DAROC fully integrated hands-on work on multiresolution tools integrated in the MuGVRE (http://gtpb.igc.gulbenkian.pt/bicourses/2018/3DAROC18/).



DATE	Title	LOCATION	Participant	Organizer	Type training	Audience size
17- 21/09/2018	3DAROC18:3C-based analysis and 3D- reconstruction of chromatin folding.	Oeiras, Portugal	CNAG-CRG	GTPB, CNAG- CRG	Hands-on MuG integrated tools + MuG VRE	14

# 3.4.1. Course description

# Course overview

3C-based methods, such as Hi-C, produce a huge amount of raw data as pairs of DNA reads that are in close spatial proximity in the cell nucleus. Overall, those interaction matrices have been used to study how the genome folds within the nucleus, which is one of the most fascinating problems in modern biology. The rigorous analysis of those paired-reads using computational tools has been essential to fully exploit the experimental technique, and to study how the genome is folded in space. Currently, there is a clear expansion on the wealth of data on genome structure with the availability of many datasets of Hi-C experiments down to 1Kb resolution (see for example: http://hic.umassmed.edu/welcome/welcome.php;

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http://promoter.bx.psu.edu/hi-c/view.php or http://www.aidenlab.org/data.html). In this course, participants will learn to use TADbit, a software designed and developed to manage all dimensionalities of the Hi-C data:

- 1. 1D Map paired-end sequences to generate Hi-C interaction matrices
- 2. 2D Normalize matrices and identify constitutive domains (TADs, compartments)
- 3. 3D Generate populations of structures which satisfy the Hi-C interaction matrices
- 4. 4D Compare samples at different time points

Participants can bring specific biological questions and/or their own 3C-based data to analyze during the course. At the end of the course, participants will be familiar with the TADbit software and will be able to fully analyze Hi-C data. On the last day, in order to be able to look beyond kb resolution in genome dynamics, participants will be introduced to computational approaches needed to bridge known atomistic insights of DNA with chromosome structure information. Two models will be introduced to provide the user of the MuG VRE detail of higher level of resolution. The first model 'MC-DNA' consists of a coarse-grained model of B-DNA where DNA is represented intrinsically at base pair level with an elastic potential representing interactions between adjacent base pairs. This model allows to probe sequence-specific properties of naked B-DNA of a sequence specified by the user. This coarse-grained DNA model is extended towards kb-long chromatin chains by implementing nucleosomes between linker DNA ('Chromatin Dynamics').

# Target audience

The course design is oriented towards experimental researchers and bioinformaticians at the graduate and post-graduate levels. The last edition of this course was attended by people with different backgrounds and interested in the genome organization. Moreover, Hi-C data have recently been used in metagenomics studies to accurately cluster metagenome assembly contigs into groups that contain nearly complete genomes of each species.

It is likely that the participants to this course aim at getting involved in generating Hi-C data for chromosome structure determination or that they just want to be able to correctly interpret and analyse publicly available data.

# 3.4.2. Feedback and conclusions

The 2018 edition of 3DAROC featured hands-on training on the MuG VRE throughout the 5 training days. A specific survey was run asking participants for feedback with regards to the training on the MuG VRE. The audience was composed mostly of postdoctoral researchers (66.7%) with 16.7% of PhD students and 16.7% of senior researchers. The survey was completed



by 50% of attendees. While most responders (83%) had not been aware of the MuG VRE, after the course they all agreed to be added to the MuG community and 70% regard the MuG VRE as a useful tool in their future work (the other 30% will consider using it). The most valued features of the VRE are the simplicity of the user interface and

the integrated workflows for analysis and visualization.



Which features offered by the MuG VRE do you value the most?

Do you regard the MuG VRE as a useful tool in your future work?



**Programme** 

# 3DAROC18

## 3C-based data analysis and 3D reconstruction of chromatin folding

Course Timetable (provisional)

Mon, Sep 17 <sup>th</sup>	Da	iy #1
09:30 - 10:00	Welcome and introductions	
10:00 - 11:00	Overview on structure determination	
11:00 - 11:30	Coffee Break	
11:30 - 12:30	3D modeling of genomes and genomic domains	
12:30 - 14:00	Lunch Break	
14:00 - 15:00	Introduction to Linux and Python: the Jupyter notebook	
15:00 - 16:00	Next Generation Sequencing (NGS) and data handling	
16:00 - 16:30	Tea Break	
16:30 - 18:00	From raw data to Hi-C contact matrices	
Tue, Sep 18 <sup>th</sup>	Da	iy #2
09:30 - 11:00	Morning wrap-up: what have we done so far? Chromatin structure and Hi-C data	
11:00 - 11:30	Coffee Break	
11:30 - 12:30	Integrative modeling applied to chromatin	
12:30 - 14:00	Lunch Break	
14:00 - 16:00	Biological application (I)	
16:00 - 16:30	Tea Break	
16:30 - 18:00	Hi-C contact matrices: filtering and normalization	

Wed, Sep 19 <sup>th</sup>	C	Day #3
09:30 - 11:00	Morning wrap-up: what have we done so far? Biological applications (II)	
11:00 - 11:30	Coffee Break	
11:30 - 12:30	Compartment detection and analysis	
12:30 - 14:00	Lunch Break	
14:00 - 16:00	Topologically Associated Domains detection and analysis	
16:00 - 16:30	Tea Break	
16:30 - 18:00	Comparison between experiments	
Thu, Sep 20 <sup>st</sup>	C	Day #4
09:30 - 11:00	Morning wrap-up: what have we done so far? Biological applications (III)	
11:00 - 11:30	Coffee Break	
11:30 - 12:30	3D Modeling of real Hi-C data with TADbit (I)	
12:30 - 14:00	Lunch Break	
14:00 - 16:00	3D Modeling of real Hi-C data with TADbit (II)	
16:00 - 16:30	Tea Break	
16:30 - 18:00	Final wrap-up session	
Fri, Sep 21 <sup>th</sup>	C	Day #5
09:30 - 11:00	Morning wrap-up: what have we done so far? Multiscale Genomics: From genomes to structures	
11:00 - 11:30	Coffee Break	
11:30 - 12:30	Nucleosome positioning and Nucleosome Dynamics	
12:30 - 14:00	Lunch Break	
14:00 - 16:00	Coarse-Grained DNA	
16:00 - 16:30	Tea Break	
16:30 - 18:00	Chromatin Dynamics	

# 3.5. MuG integrated tools featured in BioExcel webinar series

Some of the tools integrated in the MuGVRE are among the tools in the training domain of the BioExcel Center of Excellence. The possibility of using the tools in their MuGVRE integrated version has been introduced in webinars given by developers of the featured tools (namely MDWeb, NAFlex and MC\_DNA). Below are the references to the webinars in which MuG has been featured:



NAFlex, a web server for the study of nucleic acid flexibility

## (20/07/2017)

https://bioexcel.eu/webinar-naflex-aweb-server-for-the-study-of-nucleicacid-flexibility/

https://youtu.be/ZTUFsFPU\_kw (min. 49:35)



# MC\_DNA: a web server for the detailed study of the structure and dynamics of DNA and chromatin fibers

(11/04/2018)

https://bioexcel.eu/webinar-mc\_dna-aweb-server-for-the-detailed-study-ofthe-structure-and-dynamics-of-dna-andchromatin-fibers-2018-04-11/

https://youtu.be/DV3JF-jDZXQ (min. 48:20)



A Memorandum of Understanding between both initiatives has been signed which will enable such collaboration in training to remain active in the future.

# 4. DEVELOPER TRAINING

Training activities targeting developers wishing to integrate tools into the MuGVRE.

# 4.1. MuG API course

A priority of the MuG VRE developing team has been to ensure that the VRE will be sustainable in the long term and updated with the latest state-of-the-art tools. As part of this commitment, the MuG tool API was developed, allowing external tool developers to integrate their own tools.

On 13th September 2018 a MuG workshop was organized with the aim to test the performance of the tool API thoroughly and to elaborate detailed training materials and focused on two areas. The first area was internal dissemination of the underlying tool API design, integration, documentation and testing. The second area was to bring on-board a limited number of external lead users of the tool API.





DATE	Title	LOCATION	Participant	Organizer	Type training	Audience size
13/09/2018	Tool integration into MuGVRE workshop	Hinxton, UK	EBI	MuG	Internal hackathon	10 (8 int/ 2 ext)

# 4.1.1. Course description

## Course overview

The Multiscale complex Genomics (MuG) Virtual Research Environment (VRE) is a workspace designed for researchers to analyse their 3D/4D genomic data. Many tools have already been integrated including TADbit/TADkit, nucleaR and pyDock, but there are always new tools being developed. The aim of the course is to provide developers within the life sciences training to be able to wrap their own analysis tools so that it can be easily integrated into the VRE.

## <u>Audience</u>

This course is aimed at researchers and software developers that would like to integrate a new data generation or analysis tools within the VRE. The course will require knowledge of the Python programming language. Experience with high performance computing clusters is not essential, but knowing about their benefits would be advantageous.

#### Syllabus, tools and resources

During the workshop participants will learn about:

- The Multi-scale complex Genomics project (MuG)
- The MuG Virtual Research Environment (VRE)
- Programming with (Py)COMPSs
- MuG Tool API for wrapping tools
- Testing your code
- Coding standards, documentation and licenses

#### Outcomes:

- How to wrap and run a tool within the COMPSs HPC environment
- How to prepare the code repository so that it can be easily integrated within the VRE



## Programme ( 9:00 am- 5:00 pm , 13th September 2018)

- Introduction to the VRE
- How to wrap a tool using the MuG Tools API
- Running the tool in a COMPSs environment
- VRE integration
- Coding standards and documentation

# 4.1.2. Feedback and conclusions

This workshop was conceived as a way for MuG developers to test the Tool wrapping API developed within the project and to produce the necessary materials that would in the future facilitate the interaction of external tool developers wishing to integrate their tools into the VRE. The event was opened to a very limited number (2) of non-MuG participants, who have acted as lead users integrating a tool in the VRE.

The materials generated and improved during the session can be found under the training section of the MuG website (<u>http://www.multiscalegenomics.eu/MuGVRE/training/</u>).



# 5. TRAINING MATERIALS

# 5.1. Technical documentation for developers

Detailed documentation on the use of the tools wrapping API allow external developers to integrate their own tools into the VRE is accessbile from the MuG website main menu:

http://www.multiscalegenomics.eu/MuGVRE/instructions/

# 5.2. Workshop training materials

Information and documentation on the MuG training courses (including training materials) are available from the training section of the MuG website (under the support area) (<u>http://www.multiscalegenomics.eu/MuGVRE/training/</u>).

# 5.3. Tutorials

As they become available, generated tutorials are being posted under the "support" section of the website :



### http://www.multiscalegenomics.eu/MuGVRE/nucleosome-dynamics/

In addition, the support section contains links to the individual tools' help into the MuG VRE

# 6. CONCLUSIONS

MuG has successfully implemented the training plan as defined at the beginning of the project. The number and nature of training activities organized has exceeded initial project targets according to the evolving needs of the project. Training on MuG VRE integrated tools has been incorporated in established courses and specific hands-on workshops on the use of the VRE (aimed at both end users and tool developers) have been organized. Materials are available for download from the MuG website.



# 7. ANNEX II: Satisfaction surveys raw answers

The raw responses collected from the MuG training courses organized during the second reporting period are compiled below.

\*Please note that personal information of participants (names and e-mail addresses) has been removed from the tables due to the public character of the deliverable.



Timestamp	Name	E-mail	Would you like to be added to the MuG community database?	Would you like to receive MuG's periodic newsletter?	What is your position?	What is your field of expertise?	What is your overall rating of the workshop?	Please rate each session of the course: [MuG VRE presentation ]
2017/11/17 4:25:12 PM GMT+1			No	No	Postdoc researcher	Bioinformatics	1	Good
2017/11/17 4:26:11 PM GMT+1			Yes	Yes	Postdoc researcher	cosmology	3	Good
2017/11/17 5:47:40 PM GMT+1			Yes	Yes	Postdoc researcher	computational chemistry	4	Excellent
2017/11/17 6:41:52 PM GMT+1			Yes	Yes	PhD student	Genomics data analysis	3	Good
2017/11/20 9:42:39 AM GMT+1			Yes	Yes	PhD student	Chromatin structure C- techniques	4	Good
2017/11/20 9:56:04 AM GMT+1			No	No	PhD student	Hi-C data	3	Average
2017/11/20 3:41:35 PM GMT+1			Yes	Yes	Postdoc researcher	Epigenetics	3	Satisfactory
2017/11/21 6:43:34 PM GMT+1			Yes	No	Postdoc researcher	Biophysics	2	Poor
2017/11/23 12:52:31 PM GMT+1			Yes	Yes	PhD student	Epigenetics, histone variants	4	Good

# 7.1. Demo workshop 15/11/2018, Barcelona



2017/11/23 12:52:57 PM GMT+1	Yes	Yes	Senior academic / principal investigator	Genomics and Genome Structure	4	Excellent
2017/11/23 2:30:11 PM GMT+1	Yes	Yes	Masters student	Cardiovascular genetics	4	Average

Please rate each session of the course: [TADbit and TADkit: Generation of Hi-C interaction matrices from Hi-C data and visualization of 3D models]	Please rate each session of the course: [Nucleosome dynamics]	How did you hear about this workshop?	Have you used any of the resources covered in the course before?	Do you intend to use the tools /resources covered in the course in your future work?	Which features offered by the MuG portal are of most interest to you?
Satisfactory	Poor	Scientific conference	I use individual tools featured in the course frequently	Yes	Integrated analysis tools and execution of analysis workflows;Common data repository, compatible with other repositories and with personal workspace;Multi- resolution browser
Good	Did not attend	Scientific conference	No, I was unaware of them.	Yes	Source for the latest news around the 3D/4D genomics community;Integrated analysis tools and execution of analysis workflows;Common data repository, compatible with other repositories and with personal workspace
Good	Good	IRB Barcelona website	No, I was unaware of them.	Yes	Source for the latest news around the 3D/4D genomics community;Multidisciplinary hub to interact with other 3D/4D genomics community members;Integrated analysis tools and execution of analysis workflows;Common data repository, compatible with other repositories and with personal workspace;Multi- resolution browser;Training and user support
Average	Did not attend	IRB Barcelona website	I am aware of the tools but never used.	Maybe	Integrated analysis tools and execution of analysis workflows
Excellent	Good	Colleagues	I use individual tools featured in the course occasionally;I use individual tools featured in the course frequently	Yes	Source for the latest news around the 3D/4D genomics community;Multidisciplinary hub to interact with other 3D/4D genomics community members;Integrated analysis tools and execution of analysis workflows;Multi- resolution browser



Good	Average	BioMed conference registration page	No, I was unaware of them.	Maybe	Multidisciplinary hub to interact with other 3D/4D genomics community members
Satisfactory	Did not attend	Colleagues	No, I was unaware of them.	Yes	Source for the latest news around the 3D/4D genomics community;Integrated analysis tools and execution of analysis workflows;Common data repository, compatible with other repositories and with personal workspace
Poor	Poor	BioMed conference registration page	No, I was unaware of them.	Yes	Integrated analysis tools and execution of analysis workflows;Common data repository, compatible with other repositories and with personal workspace;Multi- resolution browser
Good	Good	BioMed conference registration page	No, I was unaware of them.	Yes	Integrated analysis tools and execution of analysis workflows;Common data repository, compatible with other repositories and with personal workspace;Multi- resolution browser;Training and user support
Excellent	Good	Colleagues	I use individual tools featured in the course occasionally	Yes	Multidisciplinary hub to interact with other 3D/4D genomics community members;Integrated analysis tools and execution of analysis workflows;Common data repository, compatible with other repositories and with personal workspace;Multi-resolution browser;Training and user support;Potential to generate agreed standards and formats for 3D genome data
Average	Average	Scientific conference	No, I was unaware of them.	Maybe	Integrated analysis tools and execution of analysis workflows;Common data repository, compatible with other repositories and with personal workspace;Multi- resolution browser;Training and user support

Any suggestions for MuG developers to improve the VRE functionality according to your needs as a user? Are you missing any features?	Any further comments or suggestions for future MuG training activities?	Any other comments or suggestions?
The UX is terrible and has to be rethought		
	It would be better if it was hands on. If hands on not possible (as in Barcelona), then a better projector would be good.	



	In my opinion this kind of seminars with only one person with the computer is not the best way to show the powerful of the platform. Instead some seminars with the users having computers, etc.	
It would be nice to have a simple way to log in to the system and run personal scripts with data uploaded on the system.	The workshop should have been interactive. I personally find that presentations about the functionality of a website/service in the form of a slide presentation, without hands on a computer, are boring and not very useful. That's why I gave a low rating to all the sessions.	In the future make it clear whether it is a hands-on training session or a presentation. The picture that was used to advertise the workshop that showed rows of computers with people working on them was misleading.
Tissue specific comparisons f 3D structures	Not yet but I expect I will when we use the platform more intensively	I was a very enjoyed event and I look forward to being involved in the future



# 7.2. Multi-scale study of 3D chromatin structure. 2nd edition

Timestamp	Do you want to subscribe to MuG's periodic newsletter?	Can we add you to the MuG community database?	Full Name	E-mail	What is your position /career stage?
2017/12/14 5:46:02 PM GMT+1	Yes, I want to get periodic updates.	Yes, I agree.			PhD student
2017/12/14 5:52:07 PM GMT+1	Yes, I want to get periodic updates.	Yes, I agree.			PhD student
2017/12/14 6:19:20 PM GMT+1	Yes, I want to get periodic updates.	Yes, I agree.			PhD student
2017/12/14 9:25:47 PM GMT+1	Yes, I want to get periodic updates.	Yes, I agree.			Research assistant
2017/12/19 1:01:10 PM GMT+1	Yes, I want to get periodic updates.	Yes, I agree.			PhD student
2017/12/22 11:02:43 AM GMT+1	No, thank you.	Yes, I agree.			PhD student
2017/12/22 11:26:42 AM GMT+1	Yes, I want to get periodic updates.	Yes, I agree.			Masters student
2017/12/22 12:15:36 PM GMT+1	Yes, I want to get periodic updates.	Yes, I agree.			PhD student
2017/12/24 7:16:06 PM GMT+1	No, thank you.	No, thank you.			PhD student

What is your field of expertise?

What is you overall rating for the content and delivery of the course? Please rate eachPlease rate eachsession of thethecourse: [MuG VREdypresentation ]an

Please rate each session of the course: [Nucleosome dynamics: presentation and use case application]

Please rate each session of the course: [Coarse grained model of DNA. Build and analyze a sequence of interest]

Please rate each session of the course: [Coarse grained model of Chromatin. Generation and analysis of chromatin fiber structures] Please rate each session of the course: [Protein-DNA and protein-protein docking tools]



Genome Structure in meiosis	Good	Good	Good	Excellent	Excellent	Good
Protein-protein interaction						
and Protein-DNA						
interactions.	Average	Good	Good	Good	Average	Good
Bioinformatics-Structural						
Biology	Good	Good	Excellent	Excellent	Excellent	Excellent
Bioinformatics	Good	Good	Good	Good	Good	Good
	Satisfactory	Satisfactory	Satisfactory	Good	Good	Good
Nucleosoffe DNA topology	Satisfactory	Satisfactory	Satisfactory	0000	6600	0000
Cancer epigenetics	Good	Good	Good	Good	Average	Average
GENETICS	Good	Good	Excellent	Excellent	Excellent	Excellent
Chromatin Biology	Good	Excellent	Excellent	Good	Average	Average
Chromatin dynamics	Good	Good	Good	Good	Good	Good

Please rate each session of the course: [Protein-DNA interactions, DNA flexibility and binding specificity]	Please rate each session of the course: [TADbit: generation of Hi-C interaction matrices from Hi- C data]	Please rate each session of the course: [Generation of populations of structures that satisfy the Hi-C interaction matrices. Visualization of 3D models using TADkit.]	Which features offered by the MuG portal do you value the most?
Good	Excellent	Excellent	Source for the latest news around the 3D/4D genomics community;Multidisciplinary hub to interact with other 3D/4D genomics community members;Integrated analysis tools and execution of analysis workflows;Common data repository, compatible with other repositories and with personal workspace;Multi-resolution browser;Training and user support
Good	Average	Average	Integrated analysis tools and execution of analysis workflows;Common data repository, compatible with other repositories and with personal workspace;Multi-resolution browser;Training and user support



Excellent	Good	Good	Multidisciplinary hub to interact with other 3D/4D genomics community members;Integrated analysis tools and execution of analysis workflows;Multi-resolution browser
Good	Good	Good	Integrated analysis tools and execution of analysis workflows;Training and user support
Good	Satisfactory	Satisfactory	Multidisciplinary hub to interact with other 3D/4D genomics community members;Integrated analysis tools and execution of analysis workflows;Common data repository, compatible with other repositories and with personal workspace
Excellent	Average	Did not attend	Integrated analysis tools and execution of analysis workflows; Common data repository, compatible with other repositories and with personal workspace;Training and user support
Excellent	Good	Good	Source for the latest news around the 3D/4D genomics community; Multidisciplinary hub to interact with other 3D/4D genomics community members;Integrated analysis tools and execution of analysis workflows
Average	Average	Average	Integrated analysis tools and execution of analysis workflows
Good	Good	Good	Integrated analysis tools and execution of analysis workflows

What was the best part of the course?	What was the worst part of the course?	How was the balance of theoretical and practical content?	Have you used the tools used in this course before?	Do you plan to use the tools and resources covered in the course in your future work?	Would you recommend this course?
			No, I was not familiar with any of the		
The hands-on of every part	Some theoretical parts were too long	Correct balance	tools used in the course	Yes	Yes
When the things works fine.	When the things works badly in the tabit model generation.	Correct balance	Yes, I use one or more of the tools occasionally	Yes	Yes
the interaction with other researchers from different fields and the content was very intresting for me. The tool where	Maybe the schedule could be readjusted, some activities ended before as planned, and there was some		Yes, I use one or more of the tools		
related in an example project.	"free-empty" time	Correct balance	frequently	Yes	Yes



The hands-on sessions	I wouldn't say worst, but I would have preferred a bit better organisation of the time of the sessions, i.e. too much empty time between sessions	Correct halance	No, I was not familiar with any of the	Maybe	Yes
The practical part	the theoretical part of TADhit	Too theoretical	res, i use one or more or the tools	Vec	Vec
The practical part	the theoretical part of TADDit	Too theoretical	occasionally	res	res
			Yes, I use one or more of the tools		
Coarse-grained model of chromatin	TAD-bit	Correct balance	occasionally	Yes	Yes
The best part of the course was					
discovering new techniques and tools for			No, I was not familiar with any of the		
visualisation of DNA and proteins.	The food.	Correct balance	tools used in the course	Maybe	Yes
			No. I was not familiar with any of the		
The presentation	any part	Correct balance	tools used in the course	Maybe	Yes
·			Yes Luse one or more of the tools		
Ui Canahusia	Nu ele se en se dun sus ins	Convert holence		Vaa	No.
HI-C analysis	Nucleosome dynamics	Correct balance	occasionally	res	res

What tools and/or features are you missing?	Any suggestions to improve the VRE functionality and user experience?	Any suggestions to enhance the contents or delivery of future training courses?	How did you hear about this workshop?	How do you rate the overall organization of the course (registration, communication with organizers, facilities, caterings)?	Any other comments or suggestions for future MuG training courses?
			Colleagues	Excellent	
			Colleagues	Good	Please try that everything works correctly, the presentations was very good.
			Colleagues	Good	
Analyzing experiments with biological replicates, expanding the nucleosome features to support more types of NGS data, i.e. ATAC- seq, FAIRE-seq		Maybe there would be an option of people bringing small samples of their own data for the hands on (with limitations set from the organizers, like file size)	Colleagues	Good	



Any tool to work with circular DNA, although I know that's very difficult		Time to do the "problem" exercises individually and then put them together to see the results	IRB: Multidimensional Genomics: The 3D/4D organization of chromatin	Excellent	
			Colleagues	Good	
The input types' definition	The relation between VRE and the data to be loaded to VRE can be explained better i.e. the application of the VRE to the real experimental results can be emphasised more.	The application of the VRE to the real laboratory results can be explained with more examples.	IRB Barcelona website	Good	Get to know the participant more and try to integrate their scientific data/needs to VRE as an input source.
			Scientific conference	Good	
			IRB Barcelona website	Good	

# 7.3. 3DAROC18:3C-based analysis and 3D-reconstruction of chromatin folding.

Do you want to subscrib e to MuG's periodic newslet ter?	Can we add you to the MuG comm unity datab ase?	Full Name	E-mail	What is your position /career stage?	What is your field of expertise?	Had you heard about the MuG VRE before this course?	How was the balance of theoretical and practical content (regarding the MuG VRE contents only)?	Do you regard the MuG VRE as a useful tool in your future work?	Which features offered by VRE do you value the mos	r the MuG st?	Would you be interested in attending a full course specifically about the use of the MuG VRE in the near future?
Yes, I want to get periodic	Yes, I agree.			Postdoc researcher	Functional genomics in development, evolution and disease	No, I hadn't heard about the MuG VRE before the course	Correct balance	Mayb e	Simplicity of interface;Integrated ana visualization tools and exe analysis workflows	user lysis and ecution of	Maybe



updates									
Yes, I want to get periodic updates	Yes, I agree.		PhD student	molecular biology	yes, in my lab	Correct balance	Yes	Simplicity of user interface;Integrated analysis and visualization tools and execution of analysis workflows	Maybe
Yes, I want to get periodic updates	Yes, I agree.		Senior academic / principal investigator	Bioinformatic s/Systems Biology	No, I hadn't heard about the MuG VRE before the course	Correct balance	Mayb e	Simplicity of user interface;Integrated analysis and visualization tools and execution of analysis workflows;Common data repository, compatible with other repositories and with personal workspace;Multi-resolution browser	Maybe
Yes, I want to get periodic updates	Yes, I agree.		Postdoc researcher	Genome architecture, structural variation, gene regulation	No, I hadn't heard about the MuG VRE before the course	Correct balance	Yes	Simplicity of user interface;Integrated analysis and visualization tools and execution of analysis workflows	Yes
No, thank you.	Yes, I agree.		Postdoc researcher	Cell and molecular biology	No, I hadn't heard about the MuG VRE before the course	Too theoretical	Yes	Simplicity of user interface;Integrated analysis and visualization tools and execution of analysis workflows;Common data repository, compatible with other repositories and with personal workspace	Maybe
No, thank you.	Yes, I agree.		Postdoc researcher	Chromosome/ germline biology	No, I hadn't heard about the MuG VRE before the course	Correct balance	Yes	Simplicity of user interface;Integrated analysis and visualization tools and execution of analysis workflows;Training and user support	Maybe



# 8. ANNEX II: Posters, flyers and online promotion of MuG courses

#### Multi-scale simulation of 3D chromatin structure (DEMO) 8.1.





# Multi-scale Genomics workshop: Multi-scale study of 3D Chromatin structure

This short workshop will introduce delegates to the Virtual Research Environment (VRE), created by the Multi-scale complex Genomics project (MuG), to facilitate the analysis and interpretation of the 3D and 4D

The MuG VRE integrates a range of data from genome annotation to 3D folding and DNA flexibility. Recent studies have shown the role that genome organisation can play in gene expression and the VRE has been designed to

The workshop will demonstrate how to use the multi-scale features of the VRE through integrated tools for the study of Nucleosome dynamics and for the analysis of Hi-C data and visualization of 3D models.

Organizers: Modesto Orozco (IRB Barcelona), Marc Marti-Renom (CNAG-



Nottingham EMBL-EBI

# 8.2. Multi-scale study of 3D chromatin structure: 2<sup>nd</sup> edition



Coordinated by:

BARCELONA

INSTITUTE FOR RESEARCH IN BIOMEDICINE

Hosted by:

BSC

entro Nacional le Supercomputación

MuG receives funding from the

EU's H2020 programme under grant agreement No 676556.

Barcelona Supercomputing

Center

# Multi-scale Genomics workshop



II multi-scale study of 3D chromatin structure Date: 13<sup>th</sup>-14<sup>th</sup> December 2017 Venue: Barcelona Supercomputing Center Jordi Girona, 29-31, 08034 Barcelona

http://www.multiscalegenomics.eu/MuGVRE/training/

## Multi-scale study of 3D Chromatin structure:

# 2<sup>nd</sup> edition

This workshop will introduce participants to the Virtual Research Environment (VRE) created by the Multi-scale complex Genomics project (MuG), to facilitate the analysis and interpretation of the 3D and 4D structure genome.

The MuG VRE integrates a range of data from genome annotation to 3D folding and DNA flexibility. Recent studies have shown the role that genome organisation can play in gene expression and the VRE has been designed to provide a way of analysing such data.

The course will explore how to use the multi-scale features and integrated tools of the VRE through the study of real biological examples.

#### Instructors:

Modesto Orozco (IRB Barcelona) Federica Battistini (IRB Barcelona) Jürgen Walther (IRB Barcelona) Ricard Illa (IRB Barcelona) Brian Jiménez (BSC) Charles Laughton (University of Nottingham) David Castillo (CNAG-CRG)





#### MuG partners:





# 8.3. 3DAROC18: 3C-based data analysis and 3D reconstruction of chromatin folding

The Gulbenkian Training Programme in Bioinformatics



# September 17<sup>th</sup> - September 21<sup>st</sup> 2018

3C-based methods, such as Hi-C, produce a huge amount of raw data as pairs of DNA reads that are in close spatial proximity in the cell nucleus. Overall, those interaction matrices have been used to study how the genome folds within the nucleus, which is one of the most fascinating problems in modern biology. The rigorous analysis of those paired-reads using computational tools has been essential to fully exploit the experimental technique, and to study how the genome is folded in space. Currently, there is a clear expansion on the wealth of data on genome structure with the availability of many datasets of Hi-C experiments down to 1Kb resolution (see for example: http://hic.umassmed.edu/welcome/welcome.php;

http://promoter.bx.psu.edu/hi-c/view.php or http://www.aidenlab.org/data.html). In this course, participants will learn to use TADbit, a software designed and developed to manage all dimensionalities of the Hi-C data:

- 1D Map paired-end sequences to generate Hi-C interaction matrices
- 2D Normalize matrices and identify constitutive domains (TADs, compartments)
- 3D Generate populations of structures which satisfy the Hi-C interaction matrices
- 4D Compare samples at different time points

#### http://gtpb.igc.gulbenkian.pt/2018/3DAROC18





# 8.4. MuG Tool API course



# 8.5. Advertising of MuG courses in different online platforms and published news about MuG training

http://www.bioinformaticsbarcelona.eu/training/training-at-bib/39/multi-scale-study-of-3dchromatin-structure-2nd-edition





## https://www.epigenesys.eu/en/in-the-news/other-events/eventdetail/426/136/multi-scalestudy-of-3d-chromatin-structure

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#### **OTHER EVENTS**

Multi-scale study of 3D Chromatin structure

Wednesday 13 December 2017 - Thursday 14 December 2017

#### Home > In the News > Other events



#### https://www.ebi.ac.uk/training/events/2017/multi-scale-study-3d-chromatin-structure



#### Multi-scale study of 3D Chromatin structure

This workshop will introduce delegates to a Virtual Research Environment (VRE), created by the Multi-scale

This workshop will introduce delegates to a <u>virtual research Environment (vrtc)</u>, related by the Multi-Sate complex Genomics project (Mulc), to facilitate the analysis and interpretation of the genome. This environment integrates a range of data from genome annotation to 3D folding and DNA flexibility. Recent studies have shown the role that genome organisation can play in gene expression and the VRE has been designed to provide a way of analysing such data. This course will explore how to use the MuG VRE through two case studies; cohesin's role in genome organisation in yeast and the proto-oncogene DNA-binding transcription factor Ets 1. Both will show how to analyse chromatin structure, model DNA flexibility and protein-DNA interactions.

The workshop is aimed at both experimental (bench-based) researchers and bioinformaticians; additionally it may

Participants should have an undergraduate understanding of biology AND have knowledge of genome organisation

be of interest to tool developers who wish to integrate their tools into the VRE

Nucleosome dynamics Hi-C, interaction matrices and TADs (topologically associating domains)

Date: Monday 10 - Tuesday 11 April 2017
Venue: European Bioinformatics Institute (EMBL-EBI) - Wellcome Genome Campus, Hinxton, Cambridge, CB10 1SD, United Kingdom
Application opens: Wednesday February 08 2017
Application deadline: Friday March 31 2017
Participation: First come, first served
Contact: Frank O'Donnell
Registration fee: £80
Registration closed
Find other similar courses »







#### How to apply

Places for these workshops will be allocated on a first come, first served basis.

The course fee includes use of the EMBL-EBI training rooms, lunch, refreshments and a bus to and from Cambridge rail station at the start and end of each day of the workshop (accommodatio is not included).

Application deadline



Overview

Audience

and the role it can play within the nucleus

During this workshop you will learn about: The Multi-scale complex Genomics project (MuG)

 Protein-DNA interactions Outcomes

Syllabus, tools and resources

The MuG Virtual Research Environment (VRE)

MuG-H2020-EINFRA-2015-1-676556 Deliverable 2.8: Report on the MuG training programme

#### https://www.ebi.ac.uk/training/events/2018/mug-api-course



## MuG API Course

Date: Thursday 13 September 2018
Venue: European Bioinformatics Institute (EMBL-EBI) - Wellcome Genome Campus, Hinxton, Cambridge, CB10 1SD, United Kingdom
Application opens: Tuesday June 19 2018
Application deadline: Friday August 17 2018
Participation: First come, first served
Contact: Charlotte Pearton
Registration fee: £0
Registration close
End other similar courses



Overview

The Multiscale complex Genomics (MuG) Virtual Research Environment (VRE) is a workspace designed for The mainscale contains (most) virtual research christianian (Vict) is a workspace cospilation of researchers to analyse their 30/40 genomic data. Many tools have already been integrated including TADbit/TADkit, nucleaR and pyDock, but there are always new tools being developed. The aim of the course is to provide developers within the life sciences training to be able to wrap their own analysis tools so that it can be easily integrated into the VRE.

#### Audience

This course is aimed at researchers and software developers that would like to integrate a new data generation or analysis tools within the VRE. The course will require knowledge of the Python programming language. Experience with high performance computing clusters is not essential, but knowing about their benefits would be advantageous

#### Syllabus, tools and resources

During this workshop you will learn about

- The Multi-scale complex Genomics project (MuG) The MuG Virtual Research Environment (VRE)
- Programming with (Py)COMPSs MuG Tool API for wrapping tools
- Testing your code · Coding standards, documentation and licenses

#### Outcomes

During the course you will learn:



#### How to apply

In order to be considered for a place on this course applicants must do the following:

- Complete the online application form
   Submit a WORD document
- to cpearton@ebi.ac.uk containing the following:
- · 100 word description of the tool you have developed / are developing that you would like to integrate with the VRE

## https://tess.elixir-europe.org/events/multi-scale-study-of-3d-chromatin-structure



# https://www.irbbarcelona.org/en/events/multi-scale-study-of-3d-chromatin-structure-2ndedition



# https://www.bsc.es/news/events/multi-scale-study-3d-chromatin-structure-%E2%80%93-2nd-edition

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Barcelona Supercomputing Center Centro Nacional de Supercomp	putación DISCOVER BSC RESEARCH & D	DEVELOPMENT MARENOSTRUM TECH	I TRANSFER JOIN US EL	UCATION NEWS	
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	I multi-scale study of 30 Orthomatin structure Date: 33-24 December 2017 Verue: Barcelona Supercomputing Center Jordi Girona, 29-31, 08034 Barcelona		Overview	Location	
	Overview			Location	
	This workshop will introduce delegates to a Virtual Research Environment (VRE), created by the Multi-scale complex Genomics project (MuG), to facilitate the analysis and interpretation of the 3D and 4D structure of the genome.				
	The MuG VRE integrates a range of data from g that genome organisation can play in gene expr	genome annotation to 3D folding and DNA ression and the VRE has been designed to	flexibility. Recent studies h provide a way of analysing	ave shown the role such data.	
	The course will explore how to use the multi-s	scale features and integrated tools of the	MuG VRE through the study	/ of real biologica	



#### https://www.irbbarcelona.org/en/news/a-mug-of-genomics

#### In Vivo News

# A MuG of genomics



#### 31 JAN 2018

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Multiscale Complex Genomics (MuG), a European project headed by Modesto Orozco, held back-to-back workshops on the "Multi-scale study of 3D chromatin structure" in November and December. The first took place in the context of the Barcelona Biomed Conference "Multidimensional Genomics: The 3D/4D organization of chromatin", hosted in november by IRB Barcelona, and supported by BBVA Foundation. This conference gathered together more than 150 experts in the field. The second workshop was held a month later at the Barcelona Supercomputing Center.

MuG seeks to serve as a hub for the community of researchers working in 3D and 4D genomics, providing its members with access to programmes, tools, data, infrastructure and advice. To facilitate collaborative work, MuG has developed the Virtual Research

infrastructure and advice. Io facilitate collaborative work, MuG has developed the Virtual Research Environment (VRE), which integrates a range of data from genome annotation to 3D folding and DNA flexibility. The workshops seek to teach scientists about the VRE and train them how to use its multi-scale features.

See the video to learn more about Multi-scale complex Genomics (MuG) - Exploring the Genome Beyond Sequence.



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# https://www.bsc.es/news/bsc-news/release-mug-vre-the-first-ever-platform-bring-togetherall-3d4d-genomics-information

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# Release of MuG VRE, the first-ever platform to bring together all 3D/4D genomics information

15 November 2017



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✓ News

Events



Newsletter



Today, Josep Lluís Gelpí, INB's Computational Platform leader at Barcelona Supercomputing Center (BSC), launches the MuG VRE platform at the Multi-scale study of 3D Chromatin structure session. In this session, which is co-located with the Biomed Conference, the first-ever platform encompassing all stacks of genomic data in the world will be presented.

The platform has been developed as part of the European project <u>Multiscale Genomics (MuG)</u>, in which BSC participates. It represents the first platform that unifies all 3D/4D genomic data and analysis tools in a homogeneous and organised manner. MuG VRE is particularly aimed at meeting the needs of the 3D/4D genomics research community, but it is also useful to biology laboratories that use genomic data within their research. In addition, the tool is also aimed at the industrial sector, as the comprehensive database is of great value to biotechnological companies, above all to their R&D departments.

BSC's main task in this work was the creation of the computational infrastructure on which the platform is based. The centre led the development of the foundational framework to which all data and analysis tools, as well as the data visualisation software, were later added. "The MuG VRE infrastructure has been designed to allow users to concentrate on the science, hiding all the computational complexity from them," says Josep Lluis Gelpí, project coordinator at BSC.

To coincide with the MuG VRE platform <u>launch</u>, the project has released a video setting out the project and the need for the MuG platform, as well as its different functions.



