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Virtual Reality bridge between Chemistry and Cultural Heritage: the “Sala degli Stemmi” Case Study.

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Abstract. In this contribution, we present a multiscale and multidisciplinary VR architecture that aims at creating a common environment where cultural heritage and chemistry meet in order to strengthen the role already played by chemistry in the process of restoration of cultural goods. Our aim is to create a user friendly platform where experts of both fields can share data and ideas in a direct way, in order to achieve deeper insights into cultural goods combining the scientific and historical points of view. As a case study we present the 3D reconstruction of the “Sala degli Stemmi”, which is one of the two historical rooms at Palazzo della Carovana in Pisa, presenting a number of artworks that underwent a process of chemical analysis and restoration in 2012. The whole architecture has been developed using the Unity game engine, and it is usable with HTC Vive headsets. The implementation of the VR environment and the potential applications, from both the scientific and educational points of view, are discussed in some detail.

Introduction

In the last decade, Virtual Reality (VR) has emerged as a powerful tool in several fields of hard sciences and humanities and VR technologies are increasingly used in the world of academic research and industry. Since the human beings manipulate tridimensional objects in their daily life, 3D virtual environments extend users' perception and enhance the possibility of managing big amounts of heterogeneous data coming from different sources.

These new technologies also provide the means to increase the interactions between heterogeneous fields of study, like Cultural Heritage (CH) and chemistry, which have always been deeply connected, due to the fundamental role of several chemical techniques in the process of restoration of cultural heritage goods[1–4].

Cultural heritage is a cross-cutting field in which digital technology can dramatically improve different aspects, from the preservation of the physical objects and all their physical attributes to the fruition in the form of virtual reality experiences. Recent studies[5–8] show why it is important to focus not only on visual data (such as the 3D model of an artwork), but also on all the issues related to the creation, storage, and access to metadata. In this context, virtual reality plays an important role, as it offers the possibility to visualize and to interact with the virtual representation of the artwork in its original scale. At the same time, the latest developments show the increasing importance of the collaboration among different experts with heterogeneous backgrounds in order to improve the understanding of the cultural good[6,7].

On the other side, chemistry is a conceptual subject, which has always needed the support of models and representations capable of describing that microscopic world that we are unable to see. Therefore,



virtual reality plays an important role in the process of understanding a number of key chemical topics[9,10], to such an extent that several molecular viewers originally programmed for desktop systems are being upgraded for VR devices[11–15].

On these grounds, in the present contribution we propose a multiscale and multidisciplinary VR architecture (sketched in Figure 1) that aims at finding a meeting point between heterogeneous fields such as chemistry and cultural heritage. We tried to achieve this result by creating a tool for a “virtual tour” from the macroscopic to the microscopic level, as objects of different scales and of different disciplines are going to be inspected through VR devices. The proposed architecture includes: 1) a tool for the insertion of heterogeneous data sets directly on the virtual surface of the 3D model of the cultural good; 2) a virtual and realistic representation of both the artworks and their original environment, in which it is possible to integrate the collected information; 3) a software for the investigation of the results collected from the chemical analysis, performed to drive the restoration processes.

Hence, this software encourages the sharing and confrontation of ideas among experts, with the common intent of enriching the knowledge of the subject.

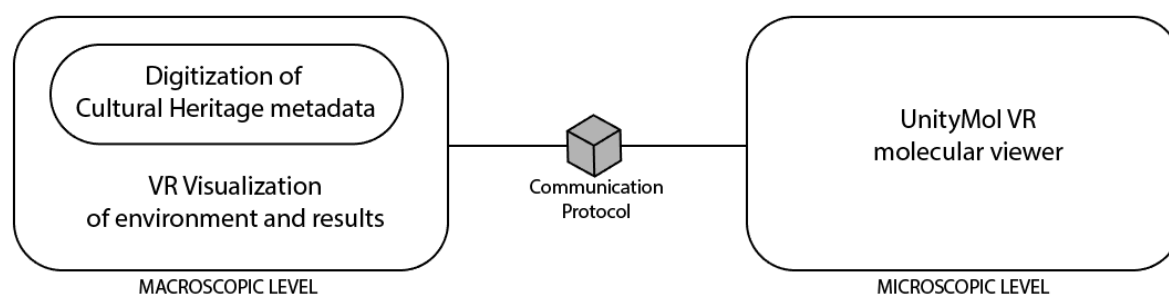


Figure 1: an overview of the different software modules that compose the architecture.

Our proof-of-concept case presents the 3D reconstruction of “Sala degli Stemmi” located at Palazzo della Carovana in Pisa. In 2012, many artworks of this historical room underwent a process of chemical analysis and subsequent restoration. To develop our VR application, a model of the room has been first realized by 3D structure from motion procedure. The architecture has been enriched with the possibility to add the sampling points of the chemical analysis and, eventually, the issuing chemical data, like composition, molecular structures and spectroscopic information. Furthermore, the user is able to visualize and interact with both the original artwork and the molecular systems identified through chemical analysis run during the restoration process.

In this architecture, a fundamental role is played by the molecular viewer. While UnityMol[15], developed using the well-known Unity cross-platform game engine [16], was initially developed only for desktop usage, its research team has recently released VR versions targeting both HTC Vive and Oculus Rift. Flexibility, expandability and modularity make UnityMol suitable for the creation of a multi-disciplinary tool, which is able to provide heterogeneous information. In the framework of an ongoing collaboration with the UnityMol team, we were able to modify the source code in order to satisfy the requirements of the sought application.

1. Related Works

Some prototypical tools have been presented in the last years, especially for the collection of heterogeneous data.

One of the first solutions has been proposed by Tsirliganis et al.[17], who focused mainly on the creation of a general database in which it is possible to store cultural and technological data for artworks. The main contribution of this study in the world of CH “is the 3D recording and mapping of physicochemical properties in the form of a GIS-like system for every Cultural Heritage Object (CHO), while the majority of existing databases are bound to a 2D world. [...] This way, the user-researcher will be able to examine CHOs from different points of view, avoiding at the same time to impose

possible strain to the actual artwork.” The fruition of the CHO is possible through a conjunct Virtual Reality Model Language (VRML) and Java solution, which nowadays is considered obsolete.

The proposal presented by Meyer et al.[18] is based on open-source software modules for the development of a virtual reality environment for the exploitation of intra-site Cultural Heritage data, which makes it possible to explore and analyze data both at spatial and temporal levels. In this case as well, the proposed VR interaction takes advantage of a web solution, called X3D.

A few years ago, Barone et al.[6] proposed RICH, an architecture conceived and developed at the Scuola Normale Superiore. This represented the first step toward the creation of a unified framework for collecting, promoting and sharing cultural heritage data. Within this architecture, the Virtual Reality Module (VRM) supports a broad variety of virtual reality and stereoscopic display devices. However, the possibility to investigate the microscopic data directly from the macroscopic level was not explored.

Finally, Scopigno and Dellepiane [7] presented an interesting collection of tools for integration and analysis of sampled data. The SICAR software, based both on web and GIS systems, can be used to characterize the surface of the artwork, linking available knowledge to specific regions defined over it. It is a good solution for mapping information directly on the 3D surface of the artwork, however it appears to require a good expertise of the operator because of the complexity of use. The 3DHOP web software offers high-resolution single object visualizations, but it is not suited to manage complex scenes made of low-poly objects. Despite this drawback, it represents one of the most promising proposals, thanks to its availability on the web and the possibility to manage heterogeneous sets of data. To the best of our knowledge, none of the previous suggestions contemplates the use of virtual reality devices for the visualization and interaction with the artworks.

2. Implementation

Given the multiscale and multidisciplinary character of the sought application, different aspects needed to be considered, in particular:

- 1) acquisition of the point cloud to be transformed into the 3D model;
- 2) digitization of the metadata and results of chemical analysis;
- 3) integration of the digital representations inside a virtual environment;
- 4) interaction with molecular structures at the microscopic level.

In order to maintain uniformity, the whole architecture has been developed using Unity. The engine is widely used in the processes of creations of 3D experiences, including VR software. Furthermore, the Unity editor can be customizable in order to speed up application development and to execute part of code without having to run the application.

2.1. Acquisition of the 3D model

The first issue to be addressed is the acquisition of the artwork and its surroundings as a 3D model. In fact, our objective is to recreate the original environment as a whole, so that the user can visit and interact with the artwork in its primary spot. A model of the “Sala degli Stemmi” has been realized by 3D structure from motion procedure, as a result of 359 pictures shot and given as input to the Metashape [19] software.

The acquisition of the room has required four rounds of shooting, two for the walls and two for the wooden coffered ceiling. The pictures of the walls have been shot at a different angle for the upper and the lower side, and at a fixed distance, so that the images could have an overlapping side for the Metashape software to work properly. For the coffered ceiling, it has been necessary to put the camera in a perpendicular position in respect to the ceiling itself, and also to shot diagonal pictures in order to acquire also the internal part of every coffer. On the contrary, the floor has been recreated using a 3D modelling software, since its pattern is easily replicable.

Concerning the artworks to be inspected in the virtual scenario, to start we choose a wooden beam, whose colour was restored, positioned on the coffered ceiling.

2.2. Digitization

Chemical information collected during the restoration of 2012 were not digitized. All the metadata were transcribed to a PDF file. Even though our purpose is not to introduce a new standard for the targeted digitization of metadata in the cultural heritage field, we decided to enrich the architecture with the possibility to insert the results of the chemical analysis for each restored item. So, the objective of this phase is to add (or modify) new (or already existing) sample points on the 3D mesh representing the artwork.

The addition of sample points upon the virtual artefact surface requires to import the 3D model inside the virtual scene. According to a research performed some years ago [32], the total number of 3D file formats exceeds 140 units, even though only a few of them are widely used. Anyhow, each file format needs its own import algorithm. Unity, being a game engine, ensures the possibility to import different types of 3D files inside the scene during edit mode, but the source codes of these algorithms are not public, hence the source code cannot be used in play mode. It is therefore reasonable to take advantage of these algorithms by developing the sampling activity inside the edit mode. In this way, instead of setting up an executable, it will be possible to handle the sampling operations directly from the Unity engine. However, we plan to transform this part of the architecture into a stand-alone application in the future.

After importing the textured 3D mesh of the artwork inside the Unity scene, the user must add the `ImportedModel` component to the game object, as it can be seen in Figure 2. This script gives different possibilities:

- to create a new empty data container;
- to load already existing metadata;
- to add sample points directly on the surface of the mesh (see Figure 3);
- to save all sample points inside the data container;
- to export data inside a *.unitypackage* [20] (that will contain both sample points data and all the necessary scripts that another user will need in order to reproduce the same scene in its own Unity software).

The creation of a new data container is required for the insertion of new sample points.

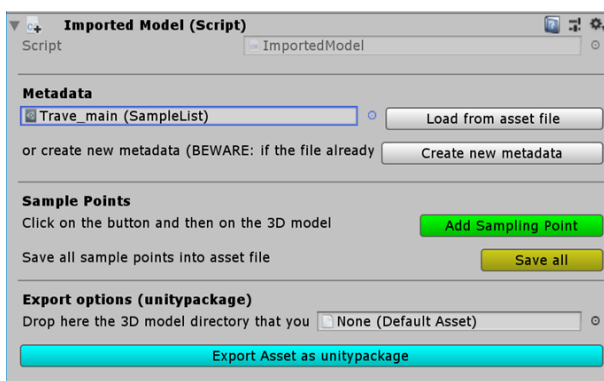


Figure 3: A screenshot of the script options when no data container has been created or loaded.

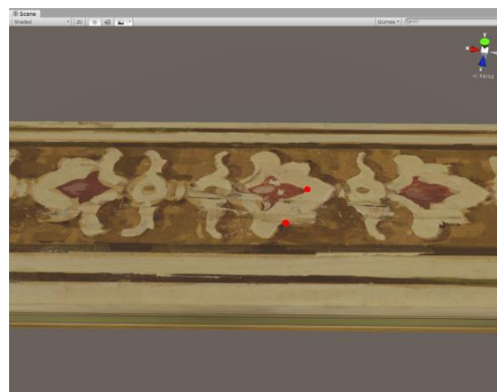


Figure 2: A screenshot of the 3D mesh of the wooden beam inside Unity Editor, showing two sample points. Each sample point is represented as a red spot on the surface of the mesh.

The data collected for each sample point are both qualitative and quantitative. In particular, each sample information will contain:

- an identification string;
- a description of the results deriving from performed chemical analysis;
- a list of the molecular structures which can be inspected in the Visualization scene.

The molecular structures can be saved as:

- SMILES[33] string;
- path of the PDB[21] file, if a structure is already available.

The SMILES notation is one of the many possible input format that Open Babel is able to read and convert into a molecular 3D structure, which will be shown in the Visualization scene. Furthermore, Open Babel can convert a SMILES notation into a PDB file, which is the requested type of input file for the UnityMol VR viewer.

The data container and the samples data are saved as a Unity asset, which are written to disk and therefore persistent between sessions.

2.3. Visualization

When the Visualization scene starts, the user finds himself standing next to the entry door of the Sala degli Stemmi. It is possible to move around by physically walking (as the Vive offers positional tracking) and by using the controller for the teleport function. In this last scenario, the player can decide to teleport only to specific predefined spots inside the virtual room. Objects of interest are highlighted with a particle system, so they are easily visible.

When an object of interest is selected, it approaches the user. At this point, the sample points are shown on the surface of the object as red spots. The user can grab the object with the controller, and open the metadata of each sample point by clicking a button on the controller and pointing directly on one of them. The metadata are shown on top of the other controller (the one not used for the selection), organized inside a panel.

When the user selects a sample point with a controller, the data of all sample points are opened and organized in a Cover Flow-like structure, as shown in Figure 4. In addition, two arrows are shown on the controller, indicating that it is possible to move between metadata by pressing the touchpad button.

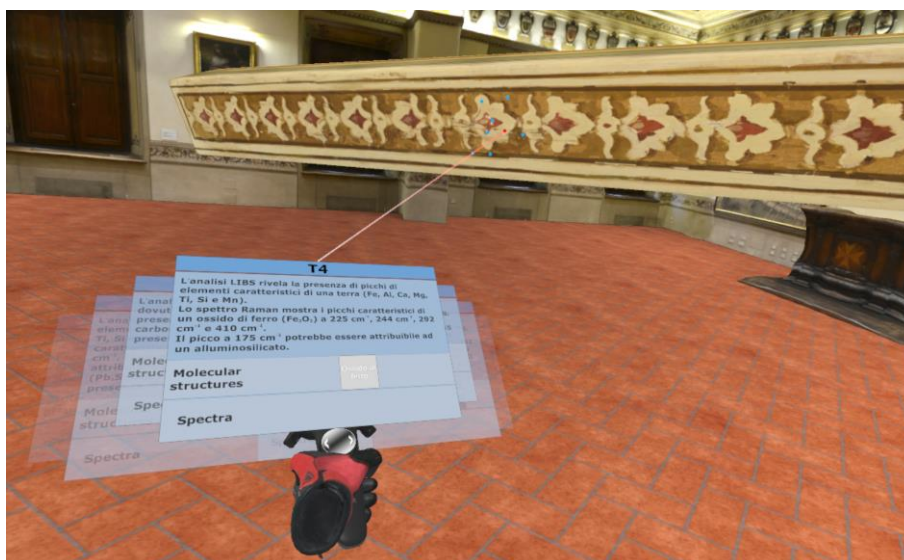


Figure 4: the object of interest (in this case, a wooden beam from the ceiling) is in front of the user. The metadata are organized in panels on the left hand of the player.

2.4. Interaction modes

In the VR visualization of Sala degli Stemmi, three types of interaction modes are available.

2.4.1. Long distance interaction. From a general point of view, two routes can be followed for allowing the user to reach far items: (i) bring the user close to the item, or (ii) bring the item in front of the user. In the first case, a possible approach would have been to move the user's virtual camera toward the item. This would have caused motion sickness, as the user's physical body movement would not match with the one in the virtual world. Another solution would have been to move instantaneously

(teleport) the player close to the item, resulting in the player floating in air. Also the latter solution has not been considered the most suitable for our scenario, and therefore option (ii) has been implemented. Once the player press a button on one of the Vive controllers, a laser beam appears. If the laser beam hits an object of interest, a circular animated timer is shown, indicating that the object will be selected in a few seconds if the laser beam stays still on it. When the selection is engaged, the object will move in front of the player.

2.4.2. Natural Interaction. Once the object is in front of the user, it is possible to interact with it in the most natural way, i.e. by grabbing it with one of the two controllers. This action lets the player inspect the whole object and its sample points. In order to do so, the player approaches the controller close to the chosen sample point, which will light up to indicate it is going to be selected. Its data are shown on a User Interface (UI) panel. Both visual and haptic feedbacks are given in order to compensate the lack of physical collision.

2.4.3. Interaction with the UI. The player can read information about the chemical analysis on a panel that has a position in the virtual world. The UI panel position is the same of the controller; hence, the player is always able to read the data without moving. This interaction is the key to the virtual trip towards the microscopic level. In fact, the player can select a molecule to be displayed by putting in contact the controller with the panel. If the virtual head of the user gets close to the opened molecule, the change of scenario is accompanied by a gentle screen fade. At this point, the state of the application is saved, so that it will be available when the player comes back from the microscopic level. Then, the user finds himself inside the UnityMol VR environment.

2.5. The communication protocol

In order to enable the exchange of messages between the upper (macroscopic) layer and the lower (microscopic) layer of the architecture, it has been necessary to implement a communication protocol. In particular, the two layers need to exchange messages about the path of the molecular file to be opened and the necessary information to switch between each other.

In our scenario, as it can be seen from Figure 1, a Client-Server model fits properly. Unity's networking has a "high-level" scripting API that, among other things, allows to control the networked state of the application, to serialize data using a general-purpose serializer, and to send and receive network messages between client (C) and server (S).

The communication protocol is composed of several scripts that are assigned to different GameObjects inside all the scenes of the project. The "Sala degli Stemmi" scene's objects include the server scripts, whereas the UnityMol scene's objects include the client scripts.

It has also been necessary to provide the following customized network messages, in particular:

- "Init" message (S → C). The server send to the client an initial message right after receiving the notification of the client connection. This message contains:
 - the PDB path of the file to be opened,
 - the name of the window and the window identifier, both necessary for switching the focus to the other application;
- "Init" message (C → S). The client sends to the server its window information as soon as they connect;
- "PDB" message (S → C). This message is sent in order to visualize a molecular structure when UnityMol is already running, as there is no need to send the windows information again.

2.6. UnityMol VR

UnityMol is a molecular viewer providing a user-friendly visualization and interaction UI developed at the Institut de Biologie Physico-Chimique (IBPC) in Paris. Among its functionalities, the latest version of the software offers Hyperballs representation[22], the possibility to load several molecules, a python console which can be used to operate on the loaded structures, and VR capabilities. [23]

UnityMol has been coded in C# inside the Unity game engine environment, which makes it easily adaptable and expandable with new features compared to similar software.

In both desktop and VR versions, UnityMol works as stand-alone application. Therefore, in order to integrate the VR version in this project, it has been necessary to adapt some features and to add new ones, such as:

- possibility to launch a UnityMol process with parameters, for example:
> UnityMol.exe -i filename.pdb
- integration of network scripts for the correct communication between “Sala degli Stemmi” VR scene and UnityMol;
- integration of functionalities for changing scenario (from/to “Sala degli Stemmi” VR scene).

When the virtual player’s head gets close to the molecule of interest inside the Visualization scene, he is “teleported” inside the UnityMol VR scenario, where the molecule is already loaded and ready to be inspected, as it can be seen in Figure 5. From this microscopic level, it is possible to go back to the macroscopic level.

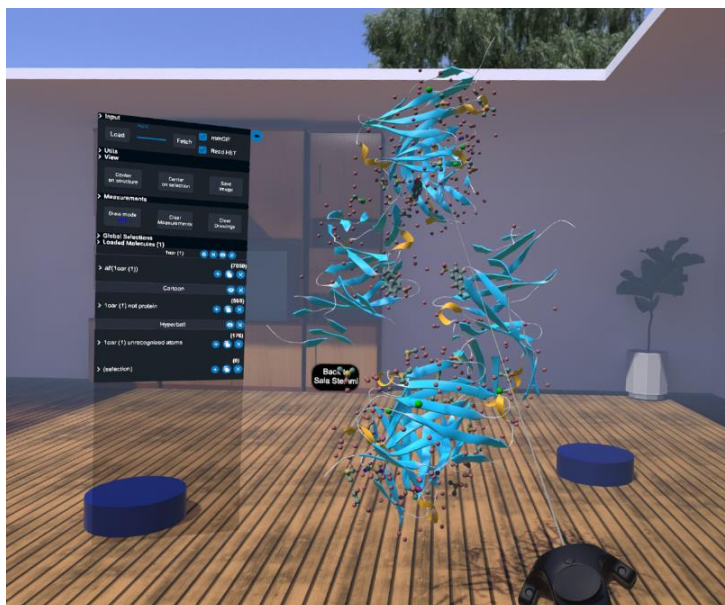


Figure 5: a screenshot of the UnityMol VR application, showing a representation of the alizarin molecule (1OAR.pdb).

3. Conclusions and future developments

In this paper, we presented the first implementation of a multiscale and multidisciplinary architecture, whose aim is to allow a “virtual trip” from the macroscopic to the microscopic level, by exploiting the virtual reality technologies. We believe that the virtual journey in VR from the macroscopic to the microscopic worlds can bring to new results and insights that would have been difficult to achieve otherwise. As future developments, we would like to integrate the possibility to visualize both molecules and crystal structures.

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References

- [1] Fantacci S, Amat A and Sgamellotti A 2010 Computational Chemistry Meets Cultural Heritage: Challenges and Perspectives *Acc. Chem. Res.* **43** 802–813

- [2] Janssens K and Grieken R V 2004 *Non-destructive Micro Analysis of Cultural Heritage Materials* (Elsevier)
- [3] Varella E A 2012 *Conservation Science for the Cultural Heritage: Applications of Instrumental Analysis* (Springer Science & Business Media)
- [4] Blümich B, Casanova F, Perlo J, Presciutti F, Anselmi C and Doherty B 2010 Noninvasive Testing of Art and Cultural Heritage by Mobile NMR *Acc. Chem. Res.* **43** 761–770
- [5] Addison A C 2001 Virtual heritage: technology in the service of culture *Proceedings of the 2001 conference on Virtual reality, archeology, and cultural heritage* (ACM) pp 343–354
- [6] Barone V, Licari D and Nardini F M 2012 RICH: Research and Innovation for Cultural Heritage *Conserv. Sci. Cult. Herit.* **12** 109–133
- [7] Scopigno R and Dellepiane M 2017 Integration and Analysis of Sampled Data: Visualization Approaches and Platforms *Sensing the Past* vol 16, ed N Masini and F Soldovieri (Cham: Springer International Publishing) pp 377–393
- [8] Pavlidis G, Koutsoudis A, Arnautoglou F, Tsioukas V and Chamzas C 2007 Methods for 3D digitization of Cultural Heritage *J. Cult. Herit.* **8** 93–98
- [9] Puzzarini C, Bloino J, Tasinato N and Barone V 2019 Accuracy and Interpretability: The Devil and the Holy Grail. New Routes across Old Boundaries in Computational Spectroscopy *Chem. Rev.* **119** 8131–8191
- [10] Licari D, Fusè M, Salvadori A, Tasinato N, Mendolicchio M, Mancini G and Barone V 2018 Towards the SMART workflow system for computational spectroscopy *Phys. Chem. Chem. Phys.* **20** 26034–26052
- [11] Salvadori A, Frate G D, Pagliai M, Mancini G and Barone V 2016 Immersive virtual reality in computational chemistry: Applications to the analysis of QM and MM data *Int. J. Quantum Chem.* **116** 1731–1746
- [12] Norrby M, Grebner C, Eriksson J and Boström J 2015 Molecular Rift: Virtual Reality for Drug Designers *J. Chem. Inf. Model.* **55** 2475–2484
- [13] Goddard T D, Huang C C, Meng E C, Pettersen E F, Couch G S, Morris J H and Ferrin T E 2018 UCSF ChimeraX: Meeting modern challenges in visualization and analysis: UCSF ChimeraX Visualization System *Protein Sci.* **27** 14–25
- [14] Wiebrands M, Malajczuk C J, Woods A J, Rohl A L and Mancera R L 2018 Molecular Dynamics Visualization (MDV): Stereoscopic 3D Display of Biomolecular Structure and Interactions Using the Unity Game Engine *J. Integr. Bioinforma.* **15**
- [15] Doutreligne S, Cragolini T, Pasquali S, Derreumaux P and Baaden M 2014 UnityMol: Interactive scientific visualization for integrative biology *2014 IEEE 4th Symposium on Large Data Analysis and Visualization (LDAV) 2014 IEEE 4th Symposium on Large Data Analysis and Visualization (LDAV)* (France: IEEE) pp 109–110
- [16] Technologies U Unity *Unity Real-Time Dev. Platf. 3D 2D VR AR Vis.*
- [17] Tsirliganis N, Pavlidis G, Koutsoudis A, Papadopoulou D, Tsompanopoulos A, Stavroglou K, Loukou Z and Chamzas C 2004 Archiving Cultural Objects in the 21st Century *J. Cult. Herit.* **5** 379–384
- [18] Meyer É, Grussenmeyer P, Perrin J-P, Durand A and Drap P 2007 A web information system for the management and the dissemination of Cultural Heritage data *J. Cult. Herit.* **8** 396–411
- [19] *Agisoft Metashape*: <https://www.agisoft.com/>. Accessed on January 2020
- [20] *Unity Manual - Asset packages*: <https://docs.unity3d.com/Manual/AssetPackages.html>. Accessed on January 2020
- [21] *PDB101 - Introduction to PDB Data*: <https://pdb101.rcsb.org/learn/guide-to-understanding-pdb-data/introduction>. Accessed on January 2020
- [22] Chavent M, Vanel A, Tek A, Levy B, Robert S, Raffin B and Baaden M 2011 GPU-accelerated atom and dynamic bond visualization using hyperballs: A unified algorithm for balls, sticks, and hyperboloids *J. Comput. Chem.* **32** 2924–2935
- [23] *UnityMol download*: <https://sourceforge.net/projects/unitymol/files/>. Accessed on January 2020.