

TileViz : Tile visualization for direct dynamics applied to astrochemical reactions.

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Abstract

We present a small multiples approach to analyze an ensemble of molecular dynamics trajectories related to reactions of astrochemical interest. A tiled visualization tool is being developed on the MANDELBROT platform housed at Maison de la Simulation in Saclay (France).

Instead of one huge screen, the TileViz software allows to present every visualization tool outputs side by side. Scientists are able to analyze multiple simulations at the same time, with varied parameters, or to visually compare similar results.

We have included in our tool the VMD molecular dynamics viewer, making it useful for the broad molecular dynamics community. Here, as a case study, we applied the approach to chemical dynamics trajectories performed by some of us with the aim of understanding possible synthetic pathways for the formation of complex organic molecules in space.

Introduction

We will present in this article a tile visualization tool with a high degree of generality and its specific application to the case study of data analysis of simulations using VMD (Visualization Molecular Dynamic) [1] on chemical reactions with astrochemical motivation. It is a small multiples approach to analyze an ensemble of chemical dynamics trajectories related to astrochemistry reactions.

When performing molecular dynamics simulations an important aspect of the results analysis is to visually perceive the atomic motions corresponding to some key events. In the case of chemical reactions, the mechanisms are the key phenomena that is often asked by the experimental community to the theoreticians. In fact, a chemical mechanism is a given sequence of atomic motions connecting reactants to products, like proton transfers, making/breaking bonds, rotational motions etc ... and all of them can be combined together in more than one possible way.

Direct dynamics is a theoretical approach which can be used to let a system react without pre-imposing any mechanism, this resulting from the physics of the model [2]. When performing direct dynamics simulations (differently to what happens in equilibrium molecular dynamics) an ensemble of trajectories are performed in order to sample the possible reaction pathways. Generally, hundreds or thousands of trajectories are used, as a function of the system, the computing power, the needed statistics, etc ... This means that one has to deal with the analysis of thousands of trajectories. A first screening can be done by employing graph theory [3, 4], from which one can distinguish the different reaction products, also in terms of isomers. In fact it is possible that the

same sequence of atoms is arranged in different ways as a product of a reaction and that they are not able to isomerize to the most stable structure (kinetic trapping). This approach was used, for example, in recent studies of unimolecular fragmentation of a number of biologically relevant molecules [5, 6], leading to the so-called theoretical mass spectra.

In the field of astro-chemistry, direct dynamics were recently used to understand the formation of complex organic molecules, like formamide [7] and glycine [8]. As result, one obtains different products which can be detected by the aforementioned graph theory tools. However, to understand in deeper details the mechanisms responsible for the different products, it was necessary to pick the different trajectories and watch the corresponding movies one by one. While this was relatively simple for formamide, for which only one product was found, it was much more complicated for glycine. In this case, a relatively large number of isomers was found as a result of two analogous reactants:



In particular, the reactions giving $H_6C_2O_2N^+ + H_2O$ are of astrophysical interest. In fact, the $H_6C_2O_2N^+$ corresponds to the brute formula of protonated glycine. Previous experiments have found that these reactions were able to form glycine, mimicking astrophysical conditions [9, 10]. Our recent simulations have confirmed that the reactions 1 and 2 provide the $H_6C_2O_2N^+ + H_2O$ products, but for $H_6C_2O_2N^+$ a number of isomers were found (eight), none of them corresponding to the structure of protonated glycine. It is thus of interest in the astrochemistry context to understand the different mechanisms leading to the products, and in particular to the three main structures found (and automatically detected by graph theory tools).

Visualization thus become an unavoidable approach to understand into details these reactions. In particular one can ask (at least) the following questions:

1. Are the mechanisms corresponding to the same reaction the same ?
2. If the same products are obtained from different reactants, are the mechanisms the same ?
3. How the mechanisms change as a function of different initial conditions, like, for example, temperature or collision energy ?

The typical visualization tools, like the widespread VMD software [1] can show only one trajectory at the same time, while

it will be useful to work with multiple trajectories, with identified flags (e.g. reactants, temperature, collision energy, method etc ...) such that in a working session one can easily access to the different information and analyze atomistic details.

VMD was developed by the Theoretical and Computational Biophysics Group in the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana-Champaign [11].

At this end we have developed a tiled visualization tool to deal with this task, which is practically employed on the MANDELBROT platform (Figure 1) housed at Maison de la Simulation in Saclay (France). Our video wall has 8K resolution of sixteen BARCO OLS-521 cubes. The video wall is stereoscopic, and we will discuss later about its application in our purposes. The wall is not tactile, but we have a 64 inches 4K tactile table that we use to interact with the video wall in full resolution (Figure 2). To support our visualization activities we have a graphical cluster with four rendering nodes bearing two NVIDIA K5000 each, then eight X11 displays in full resolution. We also have a SMP node (a symmetric shared memory multiprocessor) with 64 cores and two terabytes of memory. Finally, a video mixing system is used to extend sources from the cluster on the video wall.



Figure 1. Overview of the MANDELBROT platform: from left to right: the tactile table, a tripod for a camera, the display wall and a vertical touch screen used as a black board.



Figure 2. Mandelbrot videos wall and 64 inches tactile table

The software that we are developing is named TileViz after this type of *tiled visualization*, since it corresponds to its principal feature. Instead of one huge simulation on the screen, the TileViz software [12] allows to present every visualization tool

outputs side by side. We have included VMD molecular dynamics viewer [13] as one of the use cases to work on the chemical reaction applied to reactions of astrochemical interest (or broader to the bi-molecular reaction dynamics).

Tiled Visualization

Thanks to the improvements regarding the computing power of high-performance computing (HPC) clusters, highly demanding simulation codes (such as in molecular and direct dynamics or in modeling of global climatic phenomena) may be run with several values for each of their parameters, hence producing more precise but larger outputs. This fact implies that the methods to analyze and visualize these large databases [14] have to be adapted to their growth.

The *small multiples* visualization offers the possibility to display simultaneously a large number of graphical outputs, such as images, videos or specific software. For example, one can use a grid of simulations to compare multi-variates simulations; or large datasets with the same timescale or time steps [15], which would be tedious to analyze with all data points overlapped on a single graph.

This method has proven itself useful and complementary to other types of data visualization: in 2012, BOYANDIN *et al.* [16] compared the conclusions drawn by their subjects from the same datasets (regarding global migration flows since 1975) presented as animated images or as a grid of smaller images representing the data for each year. The findings had been similar in terms of quantity, but different in regards to the scale of the found phenomena: with animated images, the noticed patterns were short-term or short-range migration patterns, whereas the small multiples approach lead to long-term and/or large-scale findings.

However, the size of the display screen can be a major drawback to this small-multiples method [16], since the user has to find a compromise between the size of the tiles and the number of tiles on the grid.

This problem is limited or avoided with a display wall, since the surface is larger (depending of the chosen system, of course); the users do not lose resolution or image quality when they come in the room to have a work meeting. Showing numerous outputs or sub-screens is hence nicely suited to display walls.

To properly analyze multi-variates model, the dimensions are often reduced to 2 or 3; there are then tens or hundreds of 2D or 3D simulations to be printed or visualized in order to extract interesting data. These simulations may also be not images, but rather post-processing outputs straight from the computing clusters. To avoid to move large volumes of raw data, one may use only the visualized output through a remote access system, thus moving only pixel flows rather than full datasets.

Description of TileViz

TileViz may become a step or a tool in a more global workflow when processing and analyzing multi-dimensional and rich data [14]. The TileViz web client allows them to view, sort and annotate the outputs of VMD.

Use cases

The first version of TileViz is a demonstrator, but it is easily portable. Thanks to Romain Primet from INRIA Saclay, TileViz has been tested on Wilder video Wall at LRI from University

of Paris Sud, another display wall part of the DIGISCOPE cluster [17], with climate model outputs from Institut Pierre Simon Laplace Federation. In Figure 3 we show how eighty images can be displayed on the wall, arranged in eight rows. We are working on an integration of all components of this first version [18] in python, as discussed later in this paper.



Figure 3. TileViz for climate change analysis on Wilder LRI Video Wall

Moreover, the MANDELBROT room Figure 1 is fitted to host workshops or presentations, enabling work sessions with groups up to dozens of researchers, which are typically not possible in front of an individual computer.

We chose to make our software also available on classical desktop computers, since our users may wish to work on their datasets (to select interesting simulations or patterns) before their work session in the MANDELBROT room. This decision leads to the choice of Web technologies for the graphical user interface: the final user only needs to have a recent browser to launch TileViz, from their personal computer or from a larger display. For the video wall, we are currently using a dedicated browser from the WildOS suite developed at LRI.

The visualization team at Maison de la Simulation also works together with the CATI team from UNATI laboratory of CEA/Neurospin, who develops BrainVisa [19] brain analysis tool and Anatomist [20] neuroimaging tool, around tiled visualization of 3D brain scans. A case was built with them to use their anatomist [21] tool inside containers in order to handle ensemble of neuroimaging visualizations, as shown in Figure 4. To detect subtle anomalies associated with psychiatric syndromes earlier, researchers have to model the normal variability of these folds. They intend to create a dictionary of normal convolutions, from several tens of thousands of brains. To do so, they of course use automatic classification programs but they must first train these programs. This learning is based on images identified by human experts who must also validate the automatic software's first results. These experts must therefore view and compare many images in high definition, which is what TileViz allows them to do.

Features

In order to make the data analysis as easy as possible, we chose to develop simple features in our tool; they include various moves, such as swapping two tiles as in Figure 5, two lines of tiles or two columns; gathering groups of tiles with regards to their metadata or user-defined tags.

To help the visual comparison of graphs or mapped data, we coupled a drag-and-drop feature with a transparency mode, to en-

able our users to superimpose similar graphical outputs. This feature may exist generically for every simulation displayed (independently from the visualization software) thanks to some properties of the Web technologies regarding opacity of interface elements.

It is also possible to magnify one or some simulations to enhance them in high resolution and see their details more precisely as in Figure 6. In a similar way, one can also zoom on a simulation to point out a phenomenon or a pattern by drawing on the output using HTML5 canvasses. These drawings may be completed by user comments and tags, which supplement original metadata.

Drawings, user-improved metadata and interface settings are saved during each session, letting the user work on their data from

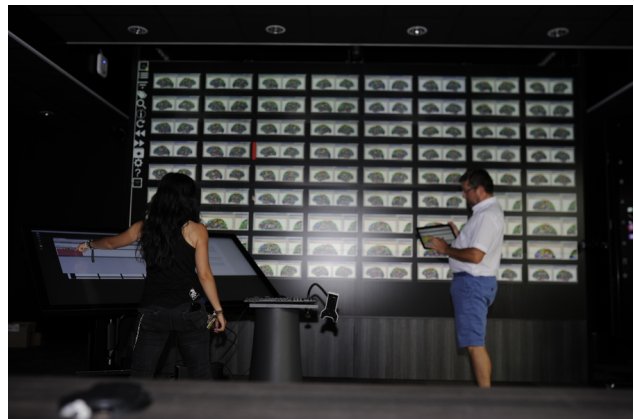


Figure 4. Working with TileViz and BrainVisa Neuroimaging tool.

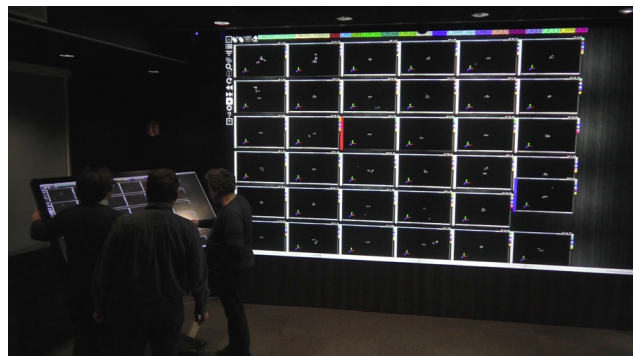


Figure 5. Moving VMD tiles on the tactile table

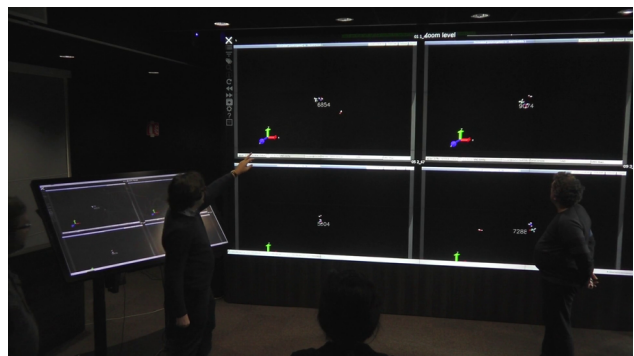


Figure 6. Time counters in zoomed mode.

various devices and explore different leads.

With our current developments to implement the existing software as a client/server application, within python Flask microframework [22], we aim to make the management of work sessions easier through databases of simulations, metadata and settings. For example, the drawings should be saved automatically in the exact configuration they were made on the tiles, and recovered when launching the next session on the regarding project.

Technical aspects

With the ever-growing computing power of HPC clusters, it has become realistic to run several simulations at the same time with different parameters, to analyze their impact even on large-scale models, such as molecular or climatic simulations. At the same time, the volume of data increases, making it more difficult to move across devices, mainly clusters and workstations.

In those conditions, we choose to use containers (namely Docker), which are lightweight virtual machines, to graphically access the simulations directly on the clusters.

Moreover, this solution has made TileViz as generic as possible thanks to the use of Docker containers. The work on the containers consists in the creation of X graphical servers, with graphical acceleration plus VNC (for Virtual Network Computing) as a remote access tool, with every graphical application needed by researchers, which in the present case corresponds to VMD. VNC is a desktop sharing server, that implements the Remote Frame Buffer protocol (RFB). It is also possible to have many containers on the same node, sharing the GPU, with a loss of performance, to increase the number of elements on the wall.

Those containers are built on a Mageia 5 Docker image (Linux distribution) with a lightweight X11 system with Xvnc (from TIGERVNC), NVIDIA driver (with the same version as the host NVIDIA driver) for graphical acceleration, and icewm as a window manager. We added x11vnc for remote access, which is compatible with noVNC [23] used in the web server of TileViz. We had to launch ntp service in start script to ensure the synchronization of the start time for some applications, and particularly the VMD for astrochemistry case described in the next part.

For security purpose, we use a generic user account at the end of the initialization process for our container. This user must have the same UID and GID than the real user that launch the containers on the cluster and we use a shared directory on a NFS network disk to manage initialization and VNC password for the launch of the viewers.

The containers may be remotely deployed on a graphical cluster linked to the supercomputer processing the numerical simulations; the running applications (like VMD) are exported to our application (running locally on the wall) through SSH tunnels with VNC stream redirections; these tunnels are also used to modify the scripts or parameters of the visualization tool. In term of performance, the application sees all the cores of the host, but we can limit the number of cores for each one. The vector acceleration in Intel processors (SSE 1 and 2 and AVX) is also available for the application. The memory and GPU are shared and if the framerate of the rendering is intensive, it may give some lag in the view, as discussed later.

Usually, depend on the TileViz case - the application inside the container - we use full screen mode of the application in the embedded X11 and launch it with the same script for all the tiles

to ensure the same view of the whole visualization. The number of the container is used as a parameter within the script (generally a python script) selecting the right dataset from the ensemble of simulations.

After the deployment of the containers, a script builds a Json file (XML language for data for Javascript) for the web server and gives for each tile the websocket of VNC stream and password for the connection to each container. We have added metadata to be able to recognize parameters of each element of the ensemble in front of the wall. This metadata file may be just a tabular with the names and values of different parameters of each simulation per line. A shell script analyzes this table to build the initial tags with group of factors in the Json list of tiles. This is very efficient to compare or select tiles in front of the wall and zoom on interesting ones chosen by scientists for example. This configuration file may be saved locally, edited as a text file and reused in a new session. We will add a database of sessions in future developments.

Thanks to VNC shared mode and QR codes (Quick Response code, a matrix barcode given complex URI) seen through a tablet with some Android decoder, zoomed views of any element can be displayed almost instantaneously. We have used noVNC [23] (websocket and Canvas for RFB decoding) package to place VNC output coming from the supercomputer with SSH tunneling on the web server to display tile representation of the ensemble of simulations.

TileViz running on our 8K video wall enables to visualize up to hundred of trajectories during collaborative meetings. We use WildOS [24], a suite of tools for display walls including a web browser, to deploy the web client of TileViz on our wall in full resolution, through the eight rendering X servers. It is based on node-webkit framework with Socket.io package to synchronize webkit clients on the wall with the server. The shared mode of VNC synchronizes the view of one application over multiple X servers as shown in Figure 7, and there is no need to make the grid of the tiles correspond the video wall nodes. It is very simple to sort tiles over the wall without moving the data nor the application on rendering nodes.



Figure 7. A single tile may be displayed across multiple servers.

Furthermore, we developed a multi-server tool in python for the Android remote control of VMD to be able to move synchronously any selected subset of tiles as in Figure 8. It analyzes the UDP socket events created by the tablet client and redirect them to multiple TCP sockets through SSH tunnels and a socat conversion is done inside each connected container to go back to the UDP socket for VMD connection.

Inside the container, the application has OpenGL 2.0 and GLSL shaders available, but the composite extension of the Xvnc server seems to disable the double frame buffer and the stereo mode cannot be activated yet. The GL_RENDERER is Gallium on llvmpipe inside our Docker containers, even if we have imported the NVIDIA GPU in the initialization. We have tested the recent nvidia-docker package (which overlay standard docker) with no more result on double frame buffer. We are actually working on these problems in order to enable stereoscopy within TileViz.

However, the use of stereoscopy, will bring new questions like for example : (1) When activated for the embedded application, will the stereoscopy mode improve the process of visual analysis in the case of hundreds of tiles on the Wall ? (2) Will this bring some new problems with synchronization for some tile across two screens in stereo, even if we have G-Sync NVIDIA cards, connecting all the GPUs of the graphical cluster ? (3) Is it compatible with displaying stereo sources with VNC to web clients ?

Unfortunately, the rendering of the web page has a cost that is visible for high frequency refreshment applications. We are working in optimizing the parallel view with eight webkit clients on the wall in charging only tiles visible for each client because we see a significant increase of the fps (frames shown per second) on all containers when we decrease the global number of tiles. This is not due to the containers themselves because when we use vncviewers directly on the nodes, we have a very high fps from the applications. The next client-server developments will give some optimization with the webkit viewers. But if one may use TileViz connected to a web database and a graphical cluster, there is a low limit with the number of tiles that can be displayed on a simple desktop screen.

Up to now, meetings were done in the Mandelbrot room facility by loading up to sixty simulations at the same time on our graphical cluster. We have displayed only thirty six tiles on example figures in this paper, for the sake of image simplicity.

Setting of a working session

Before a working session, it is important to arrange direct dynamics data, labeling the trajectories with meta-data. In particular, we have the following labels, which are here given with the most possible generality :

- Reactants: In the present case we have only two possibili-



Figure 8. Working on a subset of tiles from the initial ensemble.

ties, labeled Path 1 and Path 2;

- Products: Here we can distinguish the products as the preliminary analysis based on coordinates (and thus likely with graph theory) is done. In the present case we have three products, labeled Prod1, Prod2 and Prod3;
- Reaction mode: Here, we refer to typical applications done via direct dynamics. Bi-molecular or uni-molecular reactions are generally the two choices, but others can be added. In the present case we have only one way, which is the bi-molecular collision.
- Collision energy (CE): Here we refer to the case of bi-molecular collisions in which a determined amount of energy is given in the center-of-mass framework. This is a field which can in general cover all the extra energies given to the system. In our case we have the following values: 5, 25, 50 and 100 kcal/mol.
- Internal temperature: It is possible to make collisions with different values of internal temperature (i.e. rotational and vibrational) of the reactants. In the present case we have two values: 5 and 300 K.
- Impact parameter: In bi-molecular collisions one defines the impact parameter by which the two molecules collide (see Ref. [25] for details). In the present case we have the following values: 0, 0.5, 1.0, 1.5 and 2 Å.

Trajectories are then stored in tar files and listed following a sequential numeration. File format is, for the moment, the standard xyz. This is a simple ASCII file consisting of number of atoms in the first line, followed by a comment line and then the coordinates for each atom in Å arranged with first the element symbol and then the cartesian xyz coordinates. Once the first snapshot is done, the second follows without any blank line. However, since VMD is used, in principle every format which can be read by VMD can be employed.

Simulations used in the present case study corresponds to reactions 1 and 2, performed with VENUS package [26] coupled with MOPAC [27]. The semi-empirical Hamiltonian PM6-D was used. Different impact parameters, collision energies and temperatures were used, and for each set of simulations with the same parameters about 5000 trajectories were generated. More details can be found in Ref. [8] where the physical chemistry aspects of the work are shown and commented in details.

Session organization

A working session can be planned on a desktop computer, with a browser, and then brought in the high-resolution room MANDELBROT for collaborative meetings to manipulate the tiles using the WildOS tool on the wall with our tactile table through VNC connection or client-server mode, or any tablet connected to the wifi of the laboratory. Scientists are able to analyze multiple simulations at the same time, with varied parameters, or to visually compare similar results.

The docker containers are launched on our graphical cluster nodes. We use a SMP to manage connections and run the WildOS server to master the rendering nodes. Another VNC server from this node is connected on the tactile table to interact with this WildOS server or just use a TileViz session with a single browser in 4K extended to 8K with our video mixing system.

To prepare a session, the dataset must be reorganized fol-

lowing a sequential numeration. The metadata file has to be interpreted by a shell script to generate a node.js JSON file while the containers are launched. We use a repository called TileViz-Cases to enclose these files; generic code of TileViz is included in this directory without any modification. This file node.js can be saved by the web application in the local download directory of a client, while the location of tiles (or other parameters used by the application, such as tags or comments) are modified. It is then possible to use this new file in another session (as launching file), but for security reasons the connection (and VNC password) with containers are unique, and one has to let them open. Within this initialisation script, we have to build a dictionary to feed the search button of TileViz, and let the user search patterns in comment areas of tiles, which can be modified and saved during the session too.

The containers with VMD have to be prepared by programming a Python script which encapsulate the TCL (native language for VMD scripts) script of astro-chemists. This script ensures the synchronisation of the beginning of animations of the chemist trajectories and defines a callback which plots a counter of time steps (see Figure 6) when VMD is in full screen mode as in Figure 9.

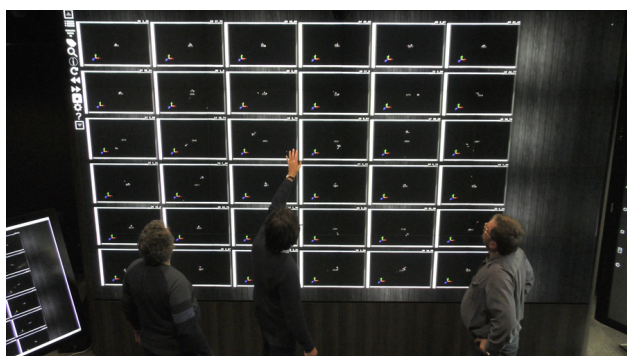


Figure 9. Full screen VMD tiles

The fullscreen mode lets the users interact only with the 3D scene, but we can suppress it for some tiles and manipulate directly the GUI of VMD, as in Figure 10.

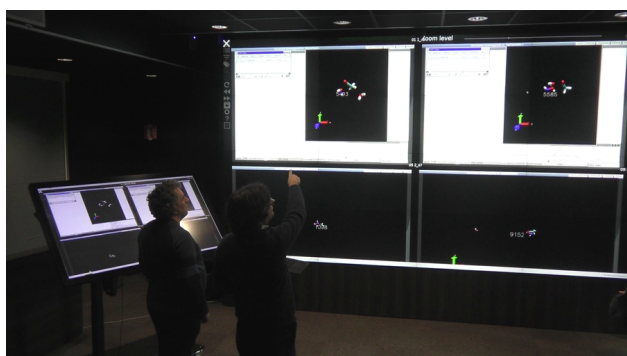


Figure 10. Access to the VMD GUI inside containers through TileViz.

Until our next version, we still launch containers by hand and we need to balance the distribution of Docker machines on the GPU nodes of the cluster, otherwise we will have important delay in VMD counters.

Conclusions and Perspectives

As a generic application TileViz opens the possibility of small multiple visualizations to plenty of research cases, and for scientists to work in a collaborative analysis setting in front of high resolution display walls. Here, we have shown a particular application in which it can be useful to visualize at the same time a relatively important number of reactive trajectories. This was applied to ion-molecule reactions which are potentially responsible to the formation of complex organic (prebiotic) molecules in space. The multiple visualization tool helps the users (which have prepared in advance the data in an appropriate way) to understand differences and analogies between an ensemble of reactive trajectories. This is important to a fine classification of the reactive events and to shed light in what are the important features for some reactions to occur.

The architecture of TileViz and its web server enable to use it along dedicated web services to view some results from simulation databases. We present here a collaboration theoretical physical chemistry researchers using VMD, a tool typical of the computational chemistry and biophysics fields, but we have already worked with some other applications specific to precise research domains, like for example, Brainvisa, developed by the CATI team from Neurospin (CEA Paris-Saclay) to study the morphology of the human cerebral cortex convolutions.

The use of containers in HPC simulations is not new and there is security problems with Docker containers. For example one is *root* (administrator account) after start container by default, which is very permissive on Linux system. The next version of TileViz will feature advanced functions such as docker compose or swarm, but we want to make it compatible to modern secure container platforms for HPC, like Kubernetes, Shifter, Singularity or CharlieCloud.

Finally, a further step will be to implement stereoscopic visualization, which will be useful, for example, when the molecular size increases, as nowadays used heavily in computational biophysics.

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Author Biography

Dr. Martial Mancip is a french research engineer from CNRS. After a PhD in Applied Mathematics, he has worked seven years with the climate French federation Institut Pierre Simon Laplace on the Orchidee continental surface model. His main accomplishment was to build a workflow to compute and monitor huge simulations of IPCC with the five coupled models. His interest for large datasets produced by HPC simulations convinced him to join Maison de la Simulation as a visualization expert in 2012 to build the Mandelbrot platform: a high resolution display wall, part of the Digiscope network of high-performance platforms for interactive visualization of large datasets and complex computations. The main developments in the visualizations team of MDLS are focused on small multiples applications for visual analysis.

Dr. Riccardo Spezia is a CNRS senior researcher. He studied at Università di Roma "La Sapienza" in Italy, where we got a PhD in theoretical physical chemistry in 2004. After a post-doctoral fellowship at Ecole Normale Supérieure - Paris (France) and Université d'Evry (France), he enrolled CNRS at Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement in Evry as junior researcher in 2006. He got the Habilitation in 2012 and recently (2017) he joined the Laboratoire de Chimie Théorique at Sorbonne Université in Paris. His interests are in the field of molecular dynamics, from force field developments for chemistry in condensed phase to reaction dynamics in the gas phase. In particular, in last years his main developments are in the field of direct dynamics for unimolecular and bi-molecular reactivity of ions leading to theoretical mass spectrometry and astrochemical reactions for the synthesis of complex organic molecules.

Dr. Yannick Jeanvoine is assistant professor in Université d'Evry (France). He studied at Université Henri Poincar'e, Nancy (France) where he received a PhD in computational and theoretical chemistry in 1998. After a post-doctoral fellowship at Technische Universität Wien (Austria), he joined the Université d'Evry at Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement (LAMBE) as assistant professor in 1999. His main interests are quantum chemical calculations and especially Density Functional Theory (DFT) which is employed to study various systems : zeolites, metal alloys, metal binding with amino acids, astrochemical reactions...

Cécile Balsier is a research engineer at Maison de la Simulation. She studied Physics and Computer Science up to a Master's degree. After an internship at Maison de la Simulation under Dr. Mancip's supervision, she joined the Visualization team to work more specifically on the development of TileViz.