Common uses of molecular visualization software in secondary school: reaching a saturation point

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Abstract: As molecular models have a growing importance in biology education, studies show that molecular visualization (MV) software can enhance the comprehension of molecular representation. But no study reports on the current common use of MV software in secondary education. This article proposes a new methodology grounded on constraints faced by educational system lying upon analysis of prescribed, potential and co-produced curricula. Part of the data collected come from the French web and Google requests done by web users. We found a reduced use of MV among biology teachers and formulate the hypothesis that this use has reached saturation. This result has been confirmed with a large set of biology and geology software, using the same methodology. Even if the methodology we used is adapted to the French context, we think it can be reused with slight adaptation in other contexts and countries.

Introduction

Because molecules are too small to be observed directly, their structures are approached with indirect techniques. X-ray crystallography is the most common technique used to get a model of the structure of a molecule. A beam of X-rays strikes a crystal of a molecule and causes a diffraction of light into many specific directions. From this pattern of diffraction, it is possible to produce a three-dimensional picture of the density of electrons within the crystal. From this electron density, the Cartesian coordinates of the atoms in the crystal can be determined. This is the process of molecular modelling. Nuclear magnetic resonance or electronic microscopy techniques are also used to create molecular models. From a particular molecular model thus obtained, it is possible to display the molecule with molecular visualization software using different types of representation.

Figure 1. The construction of a molecular model

“Structural biology has played a central role in fuelling the massive advances made by the life sciences in the last few decades” (Hodis et al., 2008, p. R121.1). Indeed, more than fifteen Nobel Prizes have been rewarded in this field since the early 50s when the DNA structure was proposed.

A great number of molecular visualization software packages are available for researchers and teachers. In 2009, Bottomley and Helmerhorst have listed at least 80 of them. Among them, RasMol was considered as the most widely used molecular visualization software around the world in the 90s (Sayle & Milner-White, 1995). More recently, it appears that Visual Molecular Dynamics (VMD) and PyMOL are widely used among researchers (Mura et al., 2010; Martz et al., 2011). PyMOL is thus, among others, regularly used to produce images that appear on the
cover page of several scientific journals, including Science and Nature (PyMOLWiki, 2012). The use of Jmol seems quite expanded, largely thanks to its easy integration into a browser. Many websites (Jmolwiki, 2012), including the Protein Data Bank (a large repository for the 3-D structural data of big biological molecules), and several scientific journals, like Nature, are using Jmol to present content in 3D.

Considering the great importance of molecular models in science and education and the fact that “three-dimensional structures are often hard to understand, even for a structural biologist”, some researchers have created an online tool, Proteopedia (http://proteopedia.org) to ease the comprehension of these structures (Hodis et al. 2008).

Literature review

What do we know about the use of Molecular Visualization software in education?

Students often have misconceptions concerning the particulate nature of matter (Harrison & Treagust, 2002; Teichert et al., 2008). Actually, this particulate nature is abstract for them (Park & Light, 2009) and conflicts with their intuitive mental models (Eilam, 2004). Students are not familiar with scientific models (Harrison & Treagust, 1996). Molecular models and representations are difficult to understand because they require some ability to visualize in a three-dimensional space (Zhang & Linn, 2011) and also some knowledge about the production process of such models (Dahmani 2009), with anchored misconceptions according to previous learning experiences (Hilton & Nichols, 2011). Textbooks, which most often include only pictures, do not provide significant resources to help students understand these representations (Gisclard, 2007).

Several studies showed that molecular visualization software can enhance the comprehension of molecular representation (Wu et al., 2001; Ferk et al., 2003; Ferk et al., 2005; Stieff, 2011; Urhahne et al., 2009). However, we made a review of the literature through the investigation of several journals (American Educational Research Journal, Biochemistry and Molecular Biology Education, Cultural Studies of Science Education, International Journal of Science and Mathematics Education, International Journal of Science Education, Journal of Research in Science Teaching, Journal of Science Education and Technology, Research in Science & Technological Education, Research in Science Education, Review of Science, Mathematics and ICT Education, Science and Education, Science Education and Studies in Science Education) and the use of the search engine “Education Resources Information Center” (ERIC) and “Google Scholar” with the following keywords “molecule”, “bioinformatics”, “science education”, “software”, “RasMol”, etc. and we didn’t find any study that investigated the global use of molecular visualization software in classrooms.

To summarize, the use of Molecular Visualization (MV) software looks interesting, but no report gives a detailed picture of current uses of this kind of software in high schools. First observations in classrooms highlighted some general difficulties using molecular visualization software: accessing files molecular (a problem that can be technically solved), taking notes while viewing a molecule, how to avoid the pitfalls associated with the molecular visualization.

Research questions

Based on this first observation, we investigated the use of molecular visualization software in the “sciences de la vie et de la Terre (SVT)” courses (i.e. biology and geology courses) in French secondary high schools. By “use”, we mean a well established and legitimate practice on a regular basis, far beyond episodic use only concerning few individuals. It can be translated by “common” use. This investigation brought us to another question: how is it possible to apprehend the use of Molecular Visualization software in education? More generally, is it possible to track the trajectory of an innovation that includes computer software and digital resources in an educational system? Answering this question leads us to search for a very specific methodology.

Methodology

The first idea would be to launch a national survey, mainly using questionnaires. But conducting such a survey can be very expensive and it is difficult to avoid some biases. Teachers may be influenced by authoritative views (for instance those of inspectors who are in charge of control in schools) and be more positive than they really
think. Anyway, questionnaire answers are declarative and it is highly time-consuming to multiply classroom observation to contrast answers and activities. Furthermore, we are interested not only to have a snapshot at one particular moment, but to get tendencies and get rationales underlying these tendencies. Concerning MV software, it is impossible to access directly to sales statistics and there are no public records of downloads.

Curricular questioning (Martinand, 2000) as a theoretical framework leads to an investigation taking into account the main features of education as a system. The overall idea is to take into account the global set of elements which have an impact on classroom practices (and therefore on the uses of MV software) on the one hand, and the global set of indices which give information about what has been done in classroom on the other hand. In other words, we want to collect the maximum of elements concerning prescribed curriculum, potential curriculum (including all elements in-between official prescription and what teachers and students will do) and co-produced curriculum (Figure 2).

**In France**

**Methodology**

Analysis from:
- Official curriculums
- Baccalaureat
- Competitive exams to recruit teachers

Inferred from:
- Interviews with teachers
- Software constraints
- Textbooks
  - Pre and in service training
  - Official websites
  - Web traces: forums, personal websites, Google queries...

Inferred from:
- Interviews with teachers
- Classroom observations
- Results about potential curriculum

**Figure 2. An overview of the methodology**

In France, there is a national curriculum that strongly constrains education. As a consequence, we investigated the official texts concerning biology teaching and made a content analysis searching for direct or indirect references to molecular visualization in the official programs from 1993 to 2012. We started with the 1993 year, because molecular visualization software became really accessible to public during this year. National examinations can also have an influence on the use of software, so we investigated the subject of the “baccalauréat” (French national examination taking place at the end of high school) from 2006 to 2011. The 2006 year was chosen because molecular visualization software begins to appear in specific tests in this year examination. And we also investigated the reports on the competitive examination used to recruit teachers in France from 2006 to 2011. Finally we reviewed the constraints inherent to the software.

There is also a whole set of hints that can be inferred from the traces left by the use of these software. We did some semi-directive interviews with six teachers considered as experts in the use of this kind of software. We investigated 25 textbooks from different editors between 1992 and 2010, tracking down references to molecular visualization. In France, the educational system is divided into 35 regional districts and every regional district has a specific website that provides educational resources for teachers. We investigated these websites in order to categorize the educational resources linked to molecular visualization software.

We sought evidence justifying the use of ICT or indicating use of ICT through an analysis of French web searches to identify sites dealing with MV software.
In France, Google is used by 90% of Internet users (AT Internet, 2010) and we made the assumption that this proportion is the same among teachers. We used Google Trends to study the most common queries of French internet users and search for MV queries. We also analyzed the queries on the website of INRP, a national institution offering a lot of resources for biology teachers and especially on molecular visualization.

We sought for other evidence in analyzing the “SVT National Forum” which is almost the only place of exchange of biology teachers on the web (“SVT National Forum” is a teachers’ association and a discussion list where near half of the total number of SVT teachers are members).

We have collected a large and heterogeneous corpus of data, quite rich but difficult to analyze. More deeply, an historical view is absolutely essential and no such historical analysis is currently available. We had to find the key actors linked to such software development in the French educational system, in order to be able to explain what were the educational goals, how the processes were launched and how their current results are seen in the educational system. Naoum Salame, a well-known pioneer of the use of software from research to secondary schools, appears to be the most important and we had an in-depth interview (two hours) with him.

**Main results**

**Constraints of molecular visualization software.** MV software can be used on subjects related to MV, which limits opportunities where they can serve. There will be therefore, a priori, one-time use of this software. For instance, in the case of DNA, MV software can be used only during one session to show the DNA structure. In addition, the software has an interface that requires a specific learning, and such learning takes time. This can be an obstacle to their use, especially in the case of occasional use, with the risk for students to forget how the software works between sessions. Finally, the scientific knowledge of the students will not use all the possibilities offered by the software, which will limit the number of possible activities with students at this level.

**Molecular visualization software are mentioned in the official curriculum.** Molecular visualization software are prescribed in the curriculum of high school for two to three labworks during each year. Over the years, the prescription has slightly varied (Figure 3).

**Molecular visualization software are mentioned in the “baccalauréat” topics** but their presence is discrete and topics that use them are very prescriptive.

Activities are almost all built on the same pattern: (1) a sequence of steps, similar to a protocol, guides the student to get some representation of the molecule, (2) he is asked to describe what he sees or to compare this representation with another one obtained previously.

In the **competition in recruiting biology and geology teachers**, mastery of MV software is expected.

**A quasi systematic presence in regional district websites.** Among the 35 regional district websites dedicated to SVT in France, 28 address the issue of the MV and mention the possible use of one or more MV software packages. 18 websites offer between 1 and 4 activities in connection with MV, to be made during labwork. The most frequent activity is the study of the structure of the DNA molecule, found in 12 sites. The proposed activities are similar to those proposed for the “baccalauréat” (high school final national examination).

Finally, it should be noticed that these websites contain only few links to the official sites of the MV software or to documentation, forums or wikis related to MV, or to the well-known encyclopaedic website *Proteopedia*.

**Textbooks**

Molecular representations are proposed in SVT textbooks since 1992. The topics covered by these textbooks are, with few exceptions, those prescribed by national curriculums (Figure 3). Most often, the textbooks of the same period and the same grade level deal with the same topics in a quite similar way. The newer textbooks are, the more molecular representations are proposed. Textbooks contain also activities that offer guided use of *RasTop*, especially in the latest ones.

These representations are, in general, pictures of a computer modelled molecular. These representations rarely exhibit a legend or a scale. Important to notice, however, is that the latest textbooks analyzed here provide more interpretable representations and sometimes give a scale. However, these representations are far from presenting all the information necessary for understanding by students and thus fostering use. Finally, the way to get these molecular models is never addressed in these books, with the exception of one. Therefore, these representations are more an illustration of a scientific paper than an element truly allowing exploitation.
Our findings support the observation made by Gisclard (2007) on French textbooks for secondary education in 2006. He stated that the 3D structures of molecules "are often shown in more decorative than educational goals" and that "the choice of mode of representation of the structure and colour indicate an almost total ignorance of the molecule in question, and a lack of pedagogical know-how (absent or meaningless or interest lacking annotations, in coordination with other documents)" (Gisclard, 2007, p. 123).

Queries related to molecular visualization on the Google search engine

The Google Insights for Search (Google, 2010) provides statistics on research conducted by Internet users worldwide on all Google sites. This service allows monitoring 5 different search terms for the period since 1 January 2004. Exploring all possible terms, we first found that generic terms like "molecular visualization", "molecule 3d", "molecule visualization", "molecular library", does not correspond to a volume of queries sufficient for the service to return results.

In contrast, significant volumes of queries correspond to more specific terms which are specific software names or acronyms. Among the most frequent, we selected the five following terms: "rasmol", "rastop", "jmol", "pymol" and "bps". RasMol, RasTop and Jmol are the only three programs mentioned in the SVT (biology and geology) official curriculums; PyMOL is widely used in research, and also in the international PDB (molecule database) repository.

Globally, the number of requests in connection with MV decreases from 2004 to 2010. Thus, the number of queries with the term "pdb" was divided by 5 to 6 during these years. The same decrease was observed in France (Figure 4).
A comparative analysis of these five terms, for the period 2004 to 2010 in France, shows that queries with the term "pdb" are 3.5 times as many queries as the term "rasmol" which place is second. Concerning only the four terms related to software applications, requests with the term "rasmol" are more frequent in 2004 while requests with "rastop" are more frequent in 2010.

We can assume that the decline of requests related to MV comes from the fact that users better know and better use available resources and thus less frequently use the search engine to get there. "pdb" queries which are placed head are probably done by researchers in biology. "rasmol" and "rastop" queries could have been made by some teachers.

**Uses and requests on the INRP national resource website.** Usable statistics are available for 2008, 2009 and 2010. The number of pages viewed in conjunction with MV has decreased, from 330,000 pages viewed in 2008, to 250,000 pages in 2010. The content of these pages has hardly changed since 2004.

**SVT National Forum:** The SVT National Forum gathers in 2011 about 8000 members (for a comparison, there are 16 541 SVT teachers in France in 2011). About 10 % (850 members) have already posted at least one message on the forum. A small core of them are interested in RasTop and, more marginally, some other in MV software like Jmol, Chime or Molusc. The major concern relative to MV software is the way to obtain molecules relevant to education.

**Few personal teachers’ websites** can be found on the web regarding MV software.

**Interviews with teachers.** The predominance of RasTop is confirmed. The discovery of MV software during training has played a role in their appropriation. Teachers discover their use and continue to use MV software to prepare labwork because they believe it improves student learning. Their labwork activities are very similar to those proposed for the high school examination (“baccalauréat”). According to them, the biggest challenge is the ability to obtain molecules.

**Classroom observations**

Two exploratory observations were made in grade 12 labwork classes in May and April 2011. During these classes, students work by handling RasTop. The purpose of these observations was to document both how the activity was conducted and how students are trying to manipulate MV software. The topics of these observations are extremely close to topics given in the national examination, with a very accurate guidance of students.

The observations showed that students seem comfortable when using MV software. They encounter no problem to start the software, or to view the molecules, to rotate them or change the structure of the molecule. But, no student was able to respond to questions about the meaning of the molecules. For example, at one question on the first observation, all students were stranded for half an hour without calling the teacher. Students do not seem to understand the meaning of the displayed molecules.

**Analysis of the conversation with Naoum Salame:** MV software have been introduced to bring the practices of science into the classes. Naoum Salame feels that the use of resources, in conjunction with MV, has changed little in the secondary education in France. He explains that these resources are consistent with official curriculums of the 2000 year and that these curriculums were modified in 2010. During this period, the themes of education that could have benefitted from 3D visualization have not changed.
Discussion

The use of molecular visualization software appears to have reached a saturation point. A rather moderate use of MV software can be observed that focuses on activities more manipulative than really conceptual. Originally, official curriculums have been introduced to bring scientific practices into the classroom. We observe a kind of "saturation", where MV software does not appear to be used as it was intended to be, and these uses remain discrete and constant over the years.

This "saturation" statement leads to several questions. In interviews or informal discussions, one element often appears in the discourse of SVT teachers: since a lot of material is available, they cannot focus on one specific kind of software. This element raise a first question: can we observe the same kind of saturation for other software applications used in SVT courses? And a second question arises from the fact that the original molecular visualization software has been introduced to promote scientific practices in the classroom.

![Diagram](image)

**Figure 5.** Most often quoted software for SVT (biology and geology), $\mathcal{S}$: not free software (other it is a free software)  
$\mathcal{L}$: software origin, $\mathcal{B}$ designed by a group or by one or two persons ( $\mathcal{B}$)

So we decided to explore the use of SVT (biology and geology) software (Figure 5) with a similar methodology. Findings are comparable to those found in the case of MV software: a saturation point is reached in the use of software in SVT classes and uses seem to occur in one or two classes during the year, in strictly guided activities. No community of teachers interested in software applications seems to appear; uses are more generally related to individual commitments.

Perspectives

How can we adapt our methodology to other countries where the educational system is not regulated in the same way? What we call curricular questioning may lead to identify main elements concerning what we call prescribed curriculum (national or state standards in US, examinations...), potential curriculum (pre and in service training, standards of institution for teacher training, textbooks, teacher communities, and so on) and co-produced curriculum and then conduct the same kind of study.
How can we follow the trajectory of an innovation in an educational system? We can see that the classical process described by Rogers (1962) is not really operational. As MV software are only occasionally used, their global use reaches a sort of plateau, and some regression can be observed.

Using “science in action” methods in secondary schools requires that students have previously acquired some competences. For example, as many tools are nowadays available, students may have many opportunities to use 3D visualization packages (3D movie and television) or glasses for augmented reality or serious games as Fold-it within a few months, and then be able to develop some visual competences leading to a better access to MV software (may in school or at home). With such new conditions, types of uses may change.

References


