Visual-auditory representation and analysis of molecular scalar fields

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Abstract

An introduction of additional sensory stimuli, mainly an auditory, in order to address a problem of visual analysis limitation is a well-known technique. We consider the problem of visual-auditory study of molecular fields and introduce an approach on the base of a concept of an abstract heterogeneous object influencing various sensory stimuli.

1 Our approach to visual-auditory scalar fields analysis

A general definition of scalar fields uses explicit functions of several variables $f(X)$, where $X = (x_1, x_2, ..., x_k)$. We treat the combination of a scalar field with its domain as a heterogeneous object that can be defined with an HyperVolume model [2], where one component is responsible for the object geometry G and other components serve as the point attribute functions representing object properties of different nature A_k such as material, color, transparency, and others that can depend on time:

$$o(t) = (G, A_c, A_t, A_s(t)) : (F(X), S_c(X), S_t(X), S_s(X|t)) \quad (1)$$

where F is a function describing geometry, S_c and S_t are attribute functions for colour and transparency that act very much like conventional transfer functions in Volume Rendering. S_s is a function describing a sound wave, an auditory attribute function that we will consider in details below.

The procedure of the mapping the scalar value, measured at the point, to the frequency (w), amplitude (a) and duration (d) leads in general to the following sound attribute function $S_s(X|t) = F_s(w(X), d(X), a(X)|t)$, where $X = (x_1.., x_n)$, t is the time.

The following mapping to a MIDI format message is considered to formalise the mapping: $(On/Off, Key, Velocity)- >(d,\ w,\ a)$. Currently, we neglect all the message components except the key number. We map scalar field value f to frequency w perceived as pitch via the following sequence of mappings:

1. To establish the mapping $f- > 0, ..N$, we calculate the scale degree $n_i \in 0, ..N$ for each scalar filed value $f(X)$ within the sub-range as $n_i = \lfloor \frac{f(X)}{\Delta d} \rfloor$, where $\Delta d = \frac{f_{max} - f_{min}}{N}$
2. $0, ..N- > MIDI_n$. The mapping for Cmaj scale of the defined range and the start key can easily be implemented on the basis of knowledge about the major scale structure of a combination of tones (T) and semi-tone (S) intervals between notes (TTSTTTS).
3. The mapping $MIDI_{Key}- > w$ can be obtained with well known MIDI keynote to the frequency conversion equation.

2 Molecular fields case study

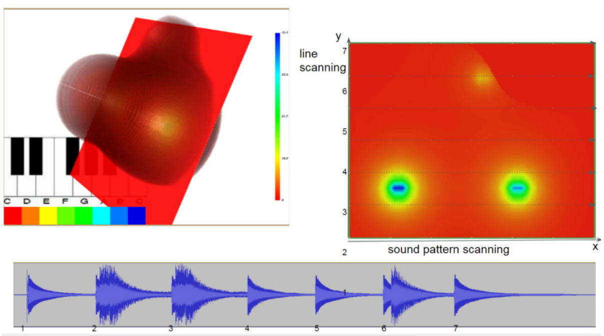

Figure 1: Exploration of HCN molecule: electron density field isosurface defines a molecule boundary, an electrostatic potential defines molecule charge property

We present a visual-auditory analysis pipeline for the molecular fields case study in quantum chemistry. The initial data is sample data from the GAMESS software package [1] that describes an HCN initial saddle point state before the HNC isomer reaction (see Fig.1 (a)). In our exploration, we have to deal with two scalar fields. The first field represents the molecule interaction boundary $(F'(X)$ (electron density field), and the second field represents the physical property, namely the charge distribution $S'_1(X)$ (see Fig.1 (b)). This leads to the molecule description in the form of a heterogeneous object:$o = (G, A_1) : (F'(X), S'_1(X))$. Via application of functional mapping procedures, that define optic and auditory transfer function, we receive a HV representation:$m(t) = (G, A_c, A_t, A_s(t)) : (F(X), S_c(X), S_t(X), S_s(X|t))$, where A_c, A_t represent an optical model and are rendered by standard Volume Rendering procedure, $S_s(X|t)$ defines sound properties and rendered along scanned path (Fig. 1 (c)).

However, in the general case of molecular fields analysis researchers have to deal with more complex dynamic case. Let us consider the process of the self-induced molecule shape optimisation [1]. In Fig.2 we present a HCCH closed shell DFT geometry optimization for the visual-auditory analysis case (sample data from GAMESS[1]). The dynamic heterogeneous object description is $o(t) = (G(t), A_c(t), A_s(t)) : (F(X|t), S_c(X|t), S_s(X|t))$, where change in time of the geometry $F(X|t)$ and the colour attribute $S_c(X|t)$ functions is modelled with the metamorphosis operation [2]. For each fixed time frame t value we obtain a molecule state description for the selected time step, that is sonified with S_s.

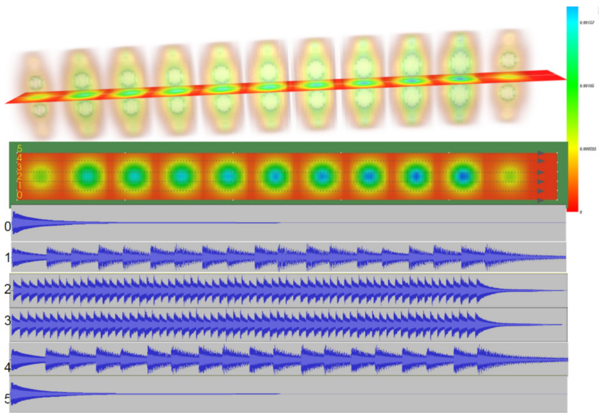

Figure 2: Exploration of the HCCH geometry optimization

Analysis of the visual and sound rendering of the scalar field slice changes in time may help to track changes in the scalar field that highlight the process of the bond type change.

3 Conclusion and further research

We have outlined the visual-auditory analysis process as a set of mappings starting with initial data sets and leading to some insight regarding scalar fields analysis. The approach is illustrated by practical case studies. Mapping into more complex music entities (chords) may provide the means for more extensive analysis of more complex data (such as a search for defects in the crystal structures). However, in some cases, an additional ear training might be even needed for researchers to be able to perceive and operate those sounds.

References

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