

# Visualization tool for comparison of mutations in protein simulations

Bruno Iochins Grisci  
Instituto de Informatica  
UFRGS  
Porto Alegre, Brazil  
Email: bigrisci@inf.ufrgs.br



Fig. 1. Teasing result of our method: from this data input (left), the relevant feature are extracted using our technique (middle), producing effective result (right).

**Abstract**—With the recent evolution of certain applications, there is a growing need for methods of this kind...

This paper proposes exactly the right solution for this sub-problem in terms of several criterions. It introduces techniques for this and that tasks, improving this characteristic of the results. It further opens to a wider range of applications, as the experiments related in this paper confirms.

**Keywords**—one or two words; separated by semicolon; from specific; to generic fields;

## I. INTRODUCTION

In the general context of this field, a certain kind of application has recently aggregated values for the following reasons. However, existing approaches to produce good results for this application do not perform optimally yet, being limited to certain aspects and requiring too much resources to be actually used.

### A. Related work

We can roughly classify the approaches used for our application in three categories: first category, second category, and last category.

Approaches in the first category were introduced by Pierre [1] using this and that techniques.



Fig. 2. Technique overview

## II. DATA CHARACTERIZATION

### A. Data dimensions

**DSSP**: The first experiment checks this aspect of our method on perfect examples.

**SASA**: The first experiment checks this aspect of our method on perfect examples.

**GYRATE**: The first experiment checks this aspect of our method on perfect examples.

**ENERGY**: The first experiment checks this aspect of our method on perfect examples.

**RMSF**: The first experiment checks this aspect of our method on perfect examples.

## III. TECHNICAL BACKGROUND

In this section, we detail this classical technique. The reader can find a more complete exposition in the work of Paul [1].

## IV. TECHNIQUE OVERVIEW

In order to produce this application, we start with this processing, followed by this technique. In order to cope with

TABLE I  
PERFORMANCES RESULTS: TIMINGS ARE EXPRESSED IN MILLISECONDS.

Data	Size	Ours	Previous	Gain
Data 1	50	0.1	1 000	$\times 10^3$
Data 2	100	0.2	2 000	$\times 10^3$
Data 3	500	0.8	10 000	$\times 10^3$
Data 4	1 000	1.2	20 000	$\times 10^3$
Data 5	5 000	1.9	100 000	$\times 10^4$
Data 6	10 000	2.1	200 000	$\times 10^4$

this challenge, we introduce this formulation to produce this intermediate result. The formulation leads to this type of system, which is efficiently solved by adapting this technique. The final result is produced by this transform. The whole process is schematized in Fig. 2.

#### A. Grid

*Item highlighting:*  
*Item selection:*

#### B. Parallel Coordinates

*Axis brushing:*  
*Axis sorting:*  
*Axis reordering:*  
*Recoloring by axis selection:*

#### C. Radar Plot

*Item highlighting:*

#### D. Slider

### V. EXPERIMENTS

We validate our technique through a series of experiments.

### VI. RESULTS AND DISCUSSION

We performed the above-mentioned experiments on the following type of data: ... For each data, we used the following tuning parameters of our method.

#### A. Performances

We report on Table I the performances of our technique on a computer at xxGhz with this graphic card. We observe that our technique outperforms previous approaches on this kind of data, and an equivalent result on this other kind of data.



Fig. 3. Quality assessment

#### B. Quality

As observed on Fig. 3, our method achieve good results in this situation. This can be measured by this criterion, and the results are reported on Table II.

TABLE II  
QUALITY MEASURES: TIMINGS ARE EXPRESSED IN MILLISECONDS.

Images	PSNR	MSE
Image 1	40.2	0.02
Image 2	30.9	1.02
Image 3	20.1	0.18

#### C. Future work

As mentioned in Section ??, we expect our method to suit better this kind of data. On the other kind, this particularity does not fit into our formulation for this and that reason. Indeed, this can be observed in the results of Fig. 3. We plan to improve for that kind of data in future work. However, our technique performed well on this data, which does not respect our condition, since this other aspect reduced the negative impact of its characteristic.

### VII. CONCLUSION

In this paper, we introduced this technique and showed that it is particularly appropriate for that application. We obtained this and that improvements, and plan to extend this application in that direction in future work.

### ACKNOWLEDGMENT

The authors would like to thank this colleague and this financing institute.

### REFERENCES

- [1] *Proceedings of the XXVIII Conference on Graphics, Patterns and Images (SIBGRAPI)*. Salvador, Brazil: IEEE, August 2015.