Report: Olav Thon foundation research funding

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Project tittle: **Complex mathematical algorithms top-down; Monte Carlo methods for path sampling explained by students for students**
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Project Period: 2016-2017-2018

In this project we improved student learning with respect to complex algorithms in molecular simulations by the development of computer based exercises and interactive visualization tools. In particular, we aimed to disseminate not only the text-book algorithms, but even the latest state-of-the-art methods, some of them being developed in the group of Prof. van Erp [1, 2]. However, we also developed dedicated exercises about more basic subjects like chaos, time-step integrators, and detailed balance in Monte Carlo.

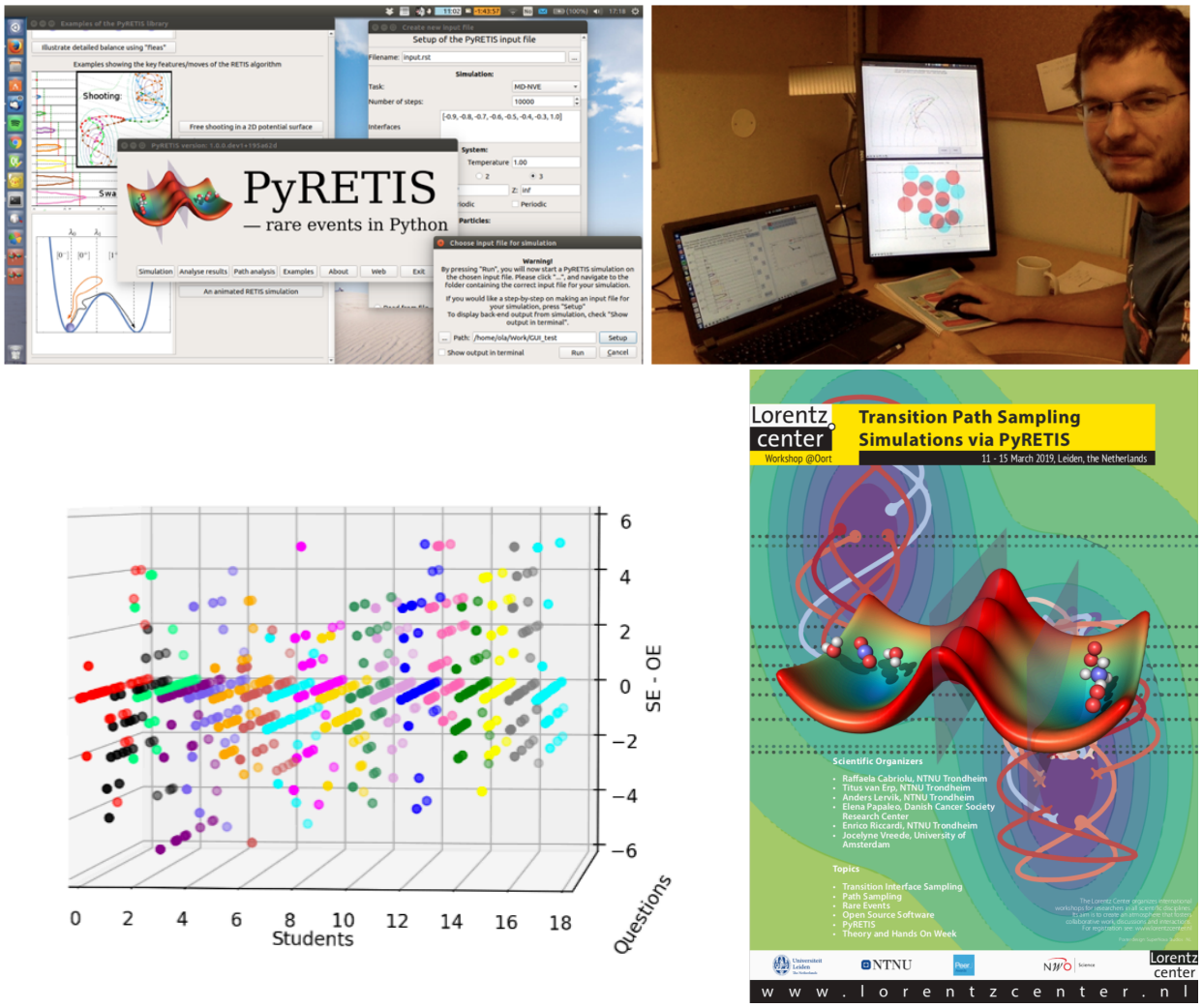

Figure 1: Top Left: Some examples of exercises shown via the GUI (Graphical User Interface). Top Right: Ola Aarøen working on the development of the GUI and the exercises. Bottom Left: a graph from the didactical paper that is presently submitted. Bottom Right: the poster of the announcement of our workshop in Leiden, the Netherlands.

In order to achieve this goal, we developed a graphical environment and integrated educational tools inside our open-source simulation package called PyRETIS (`www.pyretis.org`). These included graphical user interfaces (GUI) and real-time visualization tools. The GUIs make it very easy for students to experiment with the code since the changing parameters and getting an instant animation about the results on the screen is much more intuitive than editing an input file, read about the connection between input parameters and the statistical theories being applied, and finally having another text-file with numbers that need to be analyzed. The PyRETIS code including the educational tools got released in 2017 with a publication in the Journal of Computational Chemistry [3].

The code was first publicly demonstrated during a PhD-workshop in Mainz, Germany, for which we got an invitation by the organizers from Max Planck institute and the University of Mainz. Later, we incorporated our computer-based exercises within the NTNU master/PhD course *molecular modeling* and is now a standard part of the course that is very well appreciated. After the students worked with all kinds of interactive computer exercises, they present their findings to the other students. The fact that students work with approaches that are part of active research is highly motivating and that part is clearly reflected in the enthusiasm that the students show during their presentations.

Ola Aarøen, who developed a large part of the interactive computer tools gave a lecture about this in the seminar series of the Virtual Simulation Lab (www.virtualsimlab.com) in which PhD students explain each other about programming and visualization aspects of their work. The video of his lecture is online: https://youtube/9twqyfD_1Ac.

Oda Dahlen examined the effect of our computational exercises to the students learning outcome in a quantitative manner. Also, she examined the hypothesis whether self-evaluation is a valuable tool to differentiate and tailor the learning process to each individual students regarding skill levels and interests. The objective to that study is to establish a large database of possible exercises through which the student is guided via an algorithm. After the completion an an exercise, the algorithm should pick out the next exercise. This could be a very similar one or a very different one if the algorithm concludes that the learning target of the previous exercise was satisfactorily met. Oda presented her work on a conference in Oslo and published a paper about that study [4].

The Natural Science Faculty has realized that our initiative is something to be nurtured and have therefore gave us 250kNOK funding for our proposal VIRAL, that aims to continue the didactical innovation described above. Moreover, the Lorentz center in Leiden, the Netherlands, has hosted a PhD/postdoc school about our modeling methods and our PyRETIS computer code (https://www.lorentzcenter.nl/lc/web/2019/1106/info.php3?wsid=1106&venue=Oort). In this workshop we welcomed 42 international participants who were taught by us about theory of path sampling modeling and practical hands-on applications. The first hands-on day of the workshop was highly based on the interactive tools developed in the Olav Thon project as it gave the most intuitive introduction to the method.

References

[1] T. S. van Erp, "Reaction rate calculation by parallel path swapping.," Phys Rev Lett, vol. 98, no. 26, p. 268301, 2007.

[2] R. Cabriolu, K. M. S. Refsnes, P. G. Bolhuis, and T. S. van Erp, "Foundations and latest advances in replica exchange transition interface sampling," J. Chem. Phys., vol. 147, p. 152722, OCT 21 2017.

[3] A. Lervik, E. Riccardi, and T. S. van Erp, "PyRETIS: A well-done, medium-sized python library for rare events," J. Comput. Chem., vol. 38, no. 28, pp. 2439–2451, 2017.

[4] O. Dahlen, A. Lervik, O. Aarø en, R. Cabriolu, R. Lyng, and T. S. van Erp, "Teaching complex molecular simulation algorithms: Using self-evaluation to tailor web-based exercises at an individual level," submitted, 2019.