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The interview with the author of the PhD thesis:

„Molecular dynamics simulations of interactions between polymeric nanoparticles and lipid membranes”

Your work touches upon many distinct areas of scientific study. What caused you to give it such an interdisciplinary character?

Like every child, I was often asked: „Who do you want to be in the future?”. At that time, I always tried to answer the question unambiguously. The truth is, however, that even now, I have not arrived at a single, satisfactory answer. This is reflected in my research work, as it enables me to combine all the fields of study that interest me. I’m fortunate enough that it is my research that was inspired by my interests, and not the other way around. Therefore, the diversity in my research work results from the diversity of my interests. At the end of primary school, synthetic chemistry and growing crystals piqued my interest. Of course, at that age I was not able to (safely) carry out any major experiments, but these subjects fascinated me nonetheless. At the same time, I began learning programming, in order to create simple modifications for computer games. This also entailed learning 3D modeling (which is useful in visualizations), learning how to color them (or „texturing”, as it is known in the jargon) and learning to use programs such as GIMP or Inkscape. These foundations, along with my decision to pursue a second degree in computer science when I enrolled at university, made it much easier for me to find my way in the field of computer simulations.

What do you think posed the greatest challenge in your research?

It took me a while to come up with a good answer to this question, but I think that the biggest problem was remaining focused on what was important at a given moment. When waiting for results of your simulations, you keep coming up with ever newer and better ideas on how to solve a given problem. I often found myself thinking „this could have been solved this way”; „a slightly larger system would be useful here”; „here several smaller ones would have been more fitting”... *ad infinitum*. In extreme cases, I sometimes focused on solving completely artificial problems of my own making. Preparing and starting a simulation is a matter of a couple of days, but it takes significantly more time from an idea for a study to its publication. Due to this difference in time-scales, the design of the project, the available literature, and the understanding of the problem can change significantly. I’ve had to (rather quickly, I might add) learn to predict in advance what would be interesting and what exact settings would allow for the most efficient use of computing resources.

In what way access to Cyfronet’s supercomputing resources facilitated your research?

The word „facilitated”, in my opinion, does not fully express the impact access to these resources had on my work, as this access is what *enabled* me to carry out this research in the first place. When I started my adventure with computer simulations in 2017, I tried to use my personal computer to run the simulations. If I recall, it was technically possible to finish them, but it would have taken about 3 months, 24/7. That would have been 3 months spent on just the simulations themselves. The same simulations on a cluster (back then, it still was *Prometheus*) could have been carried out and completed in 3-4 days. That’s more than a 22-times improvement! After only 8 short years, these simulations could be successfully carried out on a fairly powerful desktop computer in a similar amount of time, by utilising graphics cards. However, technological progress makes it possible to realize greater am-

bitions for the creation of more complex and larger systems. While the preparation of systems and testing of parameters is now possible on a personal computer, Cyfronet's resources (in particular, clusters equipped with graphics cards, such as *Athena* and *Helios*) are still extremely important and needed in this field.

What are the practical applications of your research?

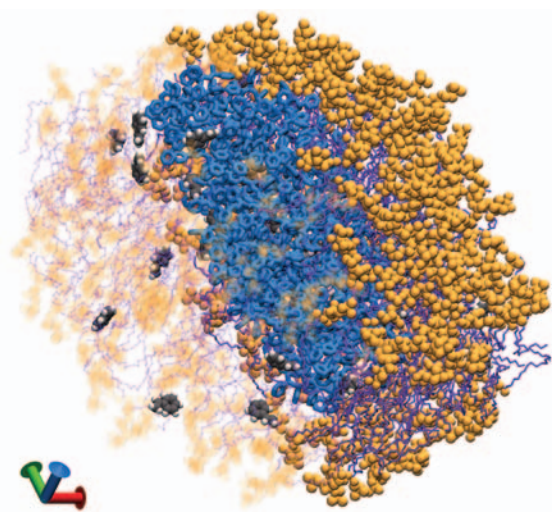
This is a fairly difficult question to answer, as my doctoral research project was conducted on many fronts. Some of them concerned polymer-based drug delivery systems based on a specific type of carriers. More specifically, it was the study of their behaviour in the presence of model cell membranes. The whole group worked on this project – people involved in experiments and simulation-oriented people, like me. My results allowed the experimental group to decide in which way to go when it comes to changes in the structure of these carriers.

The second part of my research involved nanoplastics, and in particular their ability to release the impurities contained in them, as well as pollutants adsorbed from the environment directly into cell membranes. At the time when the project was beginning, there was very little literature on this subject. At that stage, it was necessary to improve the understanding of cases in which these substances can harm us, as well as to attract more attention to the problems they pose. Our latest paper on the subject, which contains slightly extended results of this part of my PhD research, is accessed fairly often, at least according to the data received from the journal.

The last part of my research involved the development of simulation techniques themselves. Specifically, I am currently working on the development of the so-called SPICA force field, in order to add the ability to simulate systems containing sugars and glycosaminoglycans. Without going into too much detail, this technique is subtly different from those currently in use and can potentially offer more accurate results. As a part of my doctoral project, I attempted to prepare a set of parameters to facilitate this, but I have not yet received results of satisfactory quality. When the process is complete, it will significantly expand the scope of application of the SPICA force field. In addition, along with the parameterization process itself, I have created and improved many tools that will improve the work with this force field.

What advice could you give to people who are just starting their scientific careers?

By far the best advice I can offer is to focus mainly on your own personal and academic development rather than arbitrary metrics. Publishing, grants, conferences, citations – all these aspects are important for advancing one's scientific career, but in my opinion, the value of a scientist should not be judged solely based on these metrics, especially when it comes to someone who is just starting out. With a good scientific attitude and conscientious work, these „numbers“ will come naturally. Of course, one should also not forget to apply for awards for one's achievements.



Nanoplastic (polystyrene, blue lines) in a lipid membrane (orange beads and violet lines). Pollutants (in the form of residues remaining from the production process, here: styrene; shown as black and white beads) are released into the bilayer and can alter its properties.