Hi everyone, my name is Yura \*scroll\*

and my project is about the construction of surfaces of proteins. In the picture, you can see the usual representation of a protein and surfaces built from it by tools I developed. This challenge is relevant because the traditional molecular dynamics approach to docking is often too computationally expensive. And docking is essential for many vital problems of humanity such as drug design or viral dynamics. So one can try to use only surfaces of proteins for their spatial alignment, which will require way less computational power than a full molecular dynamic simulation.

Here you can read more about the solvent-excluded and solvent-accessible kinds of surfaces - the ones I’ve implemented. How they are mathematically defined and how their definitions correspond to their physical meaning. There are also original articles cited, where you can go into even more details. For now, let’s just say that the solvent-accessible surface is where centers of molecules of the solvent can go, and the solvent-excluded surface is where no part of any solvent molecules can ever be.

And here comes my project - there are currently no protein surfaces in wolfram language, so being on the wolfram summer school 2020, I thought it would’ve been nice to have them, so I’d decided to implement them in a package that is now available for any of you to download and use. Here is a one-liner import code. Having the package imported, we can pick a simple protein for the demonstration and load it from the protein databank for future use. Here is the standard cartoon view. And here is the solvent-accessible surface of our protein.

By the way, speaking of PDB-proteins, protonation is important. And now there is a wolfram-language-way to do it - a function in my package. So, this is more or less how our protein would have looked like in the real world. If you want details on protonation - algorithms are cited, and you can ask me on the live sessions of the conference or find my contacts in the description.

There are a few variable parameters, but I think we better move on now if we don’t want to break the time limit. There are two kinds of surfaces available - solvent-accessible one, which we’ve just reviewed, and the solvent-excluded one. As you can see, the latter looks less like a model from a chemistry class, but it turns out it’s very useful as well. Here, in contrast with the previous case, we get not only the 3D picture, but the whole mathematical representation on the surface. First, there is a mesh - a set of triangles, then the set of vertices the mesh was built upon, and the indices saying how to build the mesh from the given vertices. There are also a bunch of parameters you can play with. And I mean literally can - the package is out there.

But we are running out of time, so just a few words about the future possibilities. There are now many people working with protein surfaces. For example, the article I was working with is cited. There, convolutional neural networks and protein surfaces were used to dramatically speed up the docking process.

Finally, the code is published on Github, so you can see how everything works and suggest any additions for which I will be grateful.