

## Cover Letter

I have a specialization in Machine Learning and other related fields.

Also, I have developed a new **global optimization method that is better than Multistart** (without basins of attraction).

(<https://medium.com/@pushkarevvaleriyandreevich/gradient-descent-that-we-must-have-5a4542e218a0>)

Read from What to do (with gradient descent)? )

That method performs **2-3 times better than Multistart**.

And if I add basins of attractions or other optimization techniques, I will outperform even GlobalSearch and others.

Also, I have developed **a communication technique that outperforms what existed in the Linux kernel** (with a few security issues at the time).

50 million calls per second versus 5 million calls. Or more than 10 times.

(**Part 1 - Library and main concepts:**

<https://medium.com/@pushkarevvaleriyandreevich/making-libs-drivers-verilog-endpoints-for-custom-hardware-for-windows-linux-f8cf2d1e8efe>)

(**Part 2 - Hardware endpoint**

<https://medium.com/@pushkarevvaleriyandreevich/making-libs-drivers-verilog-enpoints-for-custom-hardware-for-windows-linux-8a6f580aa3f3>)

Yes, I hear that **about 3–10% improvement in one discipline is enough for a PhD**, not 2-10 times).

### Why I'm out of programming.

The basis is simple - nowadays we (humans) even have software that can program better than us (DreamCoder (DARPA)).

Also, all translation from Lisp to any language (C#/C++/Rust or even C++) can be done with Transformer (ChatGPT, etc) or analogs.

So I can say that within 2-5 years there will be no any programmer vacancy (at least in non-specialized cases).

### Why i'm in computation biology

In other hand, all basic needs (manufacturing of molecules/proteins and medicine) lies inside computational biology.

But there is a trick - we cant add unlimited number of chemical compounds to one-cell organisms forever.

(because some compound can interact with each other out of optimal reaction paths).

In many cases, we need to grow a several layer tissue to accomplish biological production of some molecules.

Also, with AlphaFold we can make almost any proteins (and validate them in quantum chemistry simulators). But it's a quite limited approach.

So studying of a growing tissues will be actual for a long time (and even connected with some manufacturing needs).

It's a material part. (I don't need to end my education without any perspectives).

### What I plan to build?

In short – A set of filters and models that will test automatically generated hypotheses (about protein functions).

For every interaction i will build a filter and a model.

Basic difference between filter and a model -

Filter should work as a bloom filter (without missing possible interactions).

Model should predict results of interactions.

I will build as many models and filters as possible.

It's quite critical to miss some possible interactions.

Also I plan to extend ways to verify all ways that protein can change its form.

So basically there is two different approaches (filters vs model as a filter)

If target is to build filters to quantum chemistry simulator:

1. Limit reaction space in simulator.

We don't need to calculate the interaction of most molecules with all proteins.

**Reaction complex is quite small.** So we can test more hypotheses and determine molecules that interact with our protein.

2. Limit reaction space part 2

Basically, protein work is a process, and **there are no molecules that can interact with the center of protein. They interact with the convex hull first.**

3. Changing of protein structure.

All changes can be approximated too.

As a base we can get a model with pH and electrons speed.

4. Ionization Zones

**Every part or protein can be ionized by light.** So we can build an ionization map based on a model of our protein.

If target is to build a protein work model (and check all possible interactions in a model):

1. Change of form during binding of molecules/ionization/temperature/pH change

2. Change of form from changing protein parts from "left/right" side of simulated protein part

Yes. That can lead to changes in electron configuration of simulated part and change its form

3. Ability to interact with external molecules (mean electric potential of protein parts)

That is connected with (1) and (2) because shape of molecule determined by electrons.

Result of work - determine functions of unknown proteins (at least what molecules can interact with it).

For that we must define **several mechanisms**:

1. Protein simply react with something and conduct reaction result
2. Specific for trans-membrane proteins – proteins change its shape and conduct electric charge
2. Protein changes its form during binding\unbinding of molecules
3. Protein changes its form during photoionization
4. Protein changes its shape during change of pH
5. Protein change its shape during change of temperature

Main hypotheses:

**Protein changes its shape during performing functions.**

**Concentrations of ions and chemical compounds are changing too.**

Combinations of those 5 mechanisms fully determine the function of protein.

Note that we can wave complex proteins that work in several steps on different basis.