Drug Discovery Project

CURRENT SITUATION

Pakistani education system fails to produce graduates with appropriate knowledge and skills required by the industry. For example, drug discovery scientists in Pakistan are trained using old text books. Students graduate with only outdated theoretical knowledge without any hands-on experience and practical knowledge of performing industrial quality lab work and using the latest software tools for drug discovery.

Engineering schools train hardware designers without giving them adequate training in using latest tools for ASIC designs and tapeout process. Similarly, software programmers are good at producing toy programs but fail to work with a large code base.

There is a serious need for planning and implementing an interdisciplinary projects to train drug discovery scientist, hardware designers and software programmers in the use of latest technologies, tools and hands-on experience to prepare them for the industry and academia.

PROPOSED SOLUTION

It is proposed that we form an interdisciplinary team consisting of drug discovery scientists, software programmers and hardware designers.

We've chosen drug discovery for our project because it involves compute-intensive calculations. This would expose our drug discovery scientists to the use of open source drug discovery tools, e.g., machine learning (TorchDrug), OpenBabel, ChemSpider, Chemical Identifier Resolver, Crystallography Open Databases, Taverna, and multiple OpenBabel applications (e.g., obminimize).

 All of the applications listed above are open source applications. All source code is available in public domain to train computer software programmers in using and making changes to a large code base. We expect programmers to be able to instrument the source code to discover compute-intensive operations that will serve as good candidates for accelerating using a new hardware.

Hardware designers will work in collaboration with the drug discovery scientists and software programmers to use the latest hardware design tools to build a hardware accelerator to speed up drug discovery calculations.

DETAILED IMPLEMENTATION PLAN

We plan to use the drug discovery process to find a cure for one or more rare diseases, also known as orphan diseases, for lack of interest by the pharmaceutical industry for economic reasons.

Examples of rare diseases include Granulomatosis with Polyangiitis (GPA) and Alkaptonuria.

We plan to use pharmaceutical scientists from Pakistani universities and laboratories, e.g., University of Health Sciences (Lahore) and Quaid-e-Azam University (Islamabad).

The role of software programmers is the key for the success of this project, they should be able to read and understand research papers, work with open source software libraries and profile the code for optimization on Hardware accelerators. Therefore, they will act like a bridge between pharmaceutical scientists and hardware engineers. They need to be proficient in C/C++ and/or different scripting languages.

The hardware designers need to work on RISC-V architecture, more specifically the vector extensions and develop hardware accelerators similar to Bit-coin miners. They should have good knowledge of Verilog hardware description language and access to Synopsys or Cadence VLSI design tools.

FINANCIAL PLAN

Initial funding required for this project: Rs. 5,000,000. per month, the commitment is for five years, but could be stopped at anytime if the required results are not achieved.

Use of proceeds includes monthly stipend to be paid to the pharmaceutical scientists, chemists, programmers and hardware designers (@ Rs. 40,000/- per month per person working for at least 20-hrs per week). Additional expenses may be incurred for purchasing chemicals, structure elucidation, characterization, and testing of biological activities.