USING QUANTUM COMPUTERS AND SUPERCOMPUTERS TO ADDRESS COVID-19 IN EGYPT (QUAN-COV-EG)

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# **QuanCovEg Project Outline**

 Motivation: COVID-19 has caused major negative impact on human life, and on economic, travel and most basic everyday life activities, locally and worldwide.

#### Project Objective:

- Building the capacity for computational drug discovery and computer-assisted epidemiological data analysis in Egypt.
  - Using the powerful computational capabilities of quantum computers (including quantum simulation) and of supercomputers (including parallel and high-performance computing).

# QuanCovEg

- Two Subprojects (Components): Drug Discovery and Epidemiological Analysis
- Drug Discovery: Simulate the chemical interaction of potential drugs with the novel coronavirus (Sars-Cov-2).
- Epidemiological Analysis: Search for factors that may speedup or slowdown the spread of the virus and the disease, and develop a model for its spread specific to Egypt.
  - Factors such as diet, weather, lockdown measures, prior vaccinations, ... etc.
  - Consider Egypt-specific factors as well as generic ones.
  - Attempt to predict the future diffusion of the virus (and disease) in Egypt.
- Both components will use the power of quantum and supercomputers, combined with that of the most recent mathematical models.
- Both components will employ artificial intelligence (AI) and machine learning (ML) methods and technologies.

# **QuanCovEg Motivating Efforts**

- In the US, sixteen (16) supercomputers are working in tandem to discover a drug for COVID-19.
  - Effort involves the US government, as well as several companies (e.g., IBM, Microsoft, Intel, and others).
  - These supercomputers are usually tasked with military research (e.g., simulations of nuclear weapons) and weather forecasting.
- In Canada, D-Wave Co. is offering **free** cloud-based access to its latest quantum computer (Leap 2.0) for COVID-19-related research.
  - D-Wave's quantum computers are specialized for performing optimization and searching algorithms. They are based on 'quantum annealing', a quantum formulation of standard simulated annealing (SA).
  - May be used also in quantum predictive analysis.
- The standard epidemiological model SIR, next to other models, is widely used by epidemiologists, locally and worldwide, to analyze the current spread of the pandemic and predict its future diffusion.

### **QuanCovEg** Tentative Team

- Myself (PI, Quantum Computing)
- Senior members:
  - Emer. Prof. Ali Hasab (Epidemiology, HIPH)
  - Emer. Prof. Muhammad Elbarrawy (Microbiology, HIPH)
  - Prof. Amr Elmasry (Algorithms, CSE Chair, Fac. of Eng.)
  - Prof. Layla AbuHadeed (Parallel/Supercomputing, CSE, Fac. of Eng.)
  - Dr. Muhammad Umar (Data Science, Visiting Scholar, EJUST-CSE)
- Junior members:
  - Eng. Ahmad Badie (Sen. SW Dev., Inova)
  - Eng. Muhammad Saad (Sen. SW Dev., Inova)
  - Eng. Amira Muhammad (Sen. SW Dev., Inova)
  - Eng. Ahmad Helmy (SW Dev., Incorta)
- (Related) Project Budget: Can it be significantly increased?
  - Discuss LATER.

#### **QuanCovEg Required Equipment**

- All main required resources are **freely** accessible, including:
  - Supercomputers.
    - Alex. Univ.
    - Informatics Research Institute, SRTA-City.
    - Arab Academy of Science and Technology (AAST).
    - All located in Alexandria governorate.
  - D-Wave's Leap 2.0 quantum computers.
    - Via cloud (i.e., Internet).

## **Project Management and Plan**

- Two teams (roughly 5 members each); a team for each component.
  - Senior members (seniors) will supervise junior members (juniors).
  - Juniors will learn and implement quantum and classical AI and ML methods and techniques suggested by the seniors.
  - PI duties:
    - In addition to active participation in the activities of each team, the PI will coordinate and facilitate communication and cooperation between members of each team.
- Two main phases:
  - Phase 1: Planning and Preparation (3-4 months).
  - Phase 2: Software Implementation and Testing (4-5 months).

## QuanCovEg Expected Outcomes

- Tried and tested knowledge and expertise among team members on how to use quantum computers and supercomputers in addressing epidemics.
- Significant findings may be patented and/or published in international journals.
  - IF any findings are reached in this short-term project.

## QuanCovEg Project Impact

- Discovering a drug for COVID-19 will have a huge impact, nationally and internationally.
- Similarly, predicting the future diffusion of the pandemic can save lives and save economies.
- Expertise in computational drug discovery and in epidemiological data analysis are valuable assets.
  - A nation that has such expertise is better equipped to deal with any current epidemics, as well as better prepared for the onset — may God forbid! — of any future ones.

# QuanCovEg Project Budget

- Currently asking for 60,000 EGP.
  - Max. allowed budget is 2,000,000 EGP in call-for-proposals announced by STIFA.
  - Project plus: Required equipment cost = 0 EGP.
- Polite request: Can incentives budget get significantly increased?
  - Still, NO salary for PI (Yes, 0 EGP!).
  - Better salaries for junior and senior members (other than PI).
    - Better dedicated; juniors will offer much more time; seniors will feel appreciation.
  - Can allow adding other team members.
    - E.g., ones from fac. of medicine, fac. of pharmacology, and fac. of engineering.
  - Increment decision is totally left to STIFA discretion.
    - Would rather NOT specify an exact figure. If pressed for some figure, then a budget of 1,000,000 EGP is definitely more than enough for all purposes.
    - If a significant increment in incentives budget is not possible, that is OK too.
      - Likely, effort will be downsized.



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