EGI-ACE Open Call no.1

3rd checkpoint meeting with shepherds

AMBER-based modelling of SARS-CoV-2 Spike protein

Shepherd: Doina Cristina Duma, Alessandro Costantini/INFN

Dissemination level:

Disclosing Party:

Recipient Party:

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Background about the scientific use case

AMBER-based modelling of SARS-CoV-2 Spike protein (1)

Overview of the scientific community representing the Data Space provider/Early Adopter use case.

- **Title:** ***"High-throughput atomistic glycan shield model of Fully-glycosylated Full-length SARS-CoV-2 Spike Protein in a Viral Membrane provides insights to design spike protein inactivators."***

Team members/organisations involved, location and type(s) of users

- **Principal Investigator**: Pasqualina D'Ursi, **Institute of Biomedical Technologies - National Research Council of Italy**
- Aditional contacts: Andrea Manconi, Alessandro Orro
- Representing an heterogeneous group of more than 11 researchers (bioinformatics, biotechnology, engineering, physics and computer science.) and 2 PhD students
- **Organizations**:
  - Institute of Biomedical Technologies of the National Research Council (**CNR-ITB**)
    - **Bioinformatics Laboratory**
  - University of Brescia (**UniBs**)
    - **Macromolecular Interaction Analysis Unit** (MIAU) in the Department of Molecular and Translational Medicine
    - New collaboration aimed at the design of compounds endowed with the capacity to block/inactivate the spike protein of the SARS- CoV2 virus
    - Doctorate project - "Design and validation of virucidal compounds for the development of anti-SARS-CoV2 Personal Protective Equipment"
  - University of Genoa (**UniGe**)
    - **Department of Pharmacy**
    - Doctorate project - "In silico methods applied on druggable proteins to identify transient pockets: new approaches for studying drug-target molecular mechanisms. A case study on CFTR."

Integration Support

- *Containerization of the analysis workflow*
- *Access to provided resources – EGI Check-in,*
  - *New research community or use an already available VO with specific sub-group*
  - *Possibility to enroll/register non IDEM users (PhD students)*
- How to use of the EGI Data transfer service, in particular for the output transfers
- ***No expertise on cloud computing***
  - access training material and/or specific training events

Capacity Requirements

Requested - access to **modern and powerful GPU** devices as well as **suitable storage and transfer data services**

10 virtual machines (VMs)
- 7 VMs dedicated to run dynamic simulations on known drug protein complexes
- 3 VMs to simulate dynamics of polyanionic polymers protein complexes

The VMs should be configured as follow:
- Image: **Centos 7** image configured to run Docker containers leveraging NVIDIA GPUs (available in the EGI applications database);
- Flavour: **2 GPU Nvidia T4, 8 cores (for GPU), 24GB RAM**;
- GPU device**: Nvidia T4 16GB** (provided by CESNET);
- Block storage: it is required a different volume for VM dedicated to simulate dynamics of (A) known drug protein complexes with respect those dedicated to simulate dynamics of ((B) polyanionic polymers protein complexes:
    - o (A): **volume of 5TB for each VM**
    - o (B): **volume of 130TB for each VM**
- **EGI Data transfer service:** volumes should be exposed to the EGI transfer service to allow easy sharing of large sets of files resulting from simulations (order of TB)

Timeline

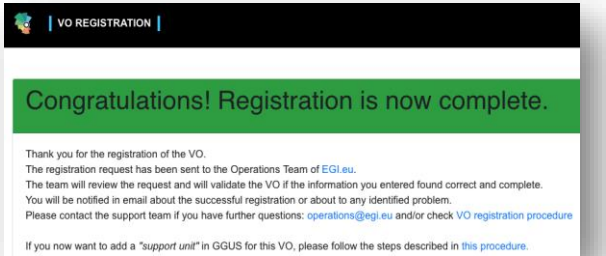
After discussing with the use-case PI

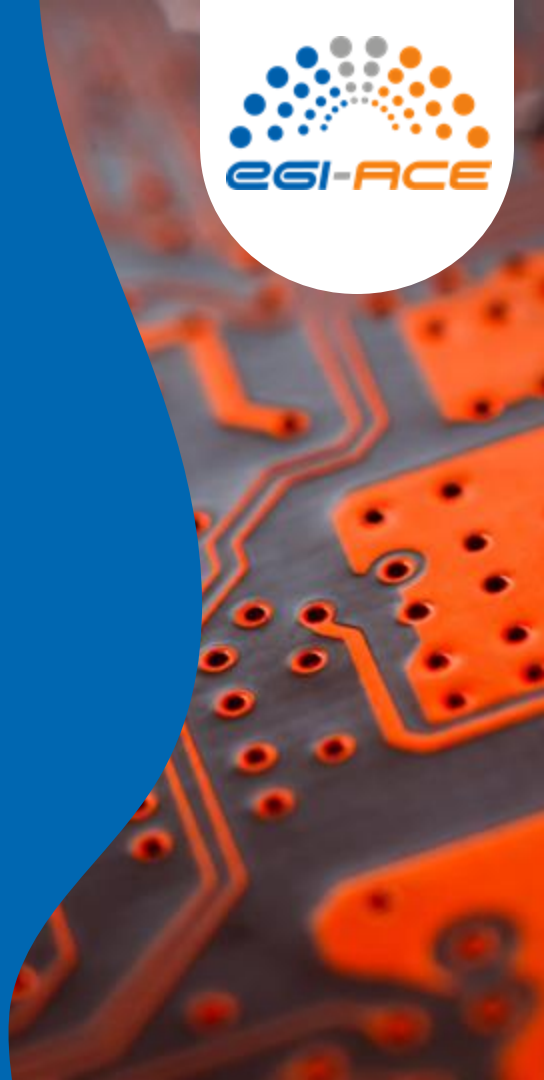
Work planned for Q1	**•Infrastructure resource provisioning and settings •Enable federated identity management using one of the available AAI solutions**
Work planned for Q2	•Tune the platform services (Compute, Data Management) •Starting molecular protocol setup and dynamic simulations on the first 7 of known drug protein complexes and on 3 polyanionic polymers protein complexes
Work planned for Q3	•Completing simulations of first 7 known drug protein complexes. •Analysis of results •Starting molecular protocol setup and dynamic simulations on the second set of 7 known drug protein complexes
Work planned for Q4	•Completing simulations on polyanionic polymers protein complexes •Completing simulations on second set of known drug protein complexes •Analysis of results

Status

As of today

- **Infrastructure resource provisioning and settings**
  - After discussing with WeNMR people the use of the AMBER portal was not feasible (not enabled for cloud usage)
  - CESNET (Miroslav) didn't answer to the request to support the use-case, as stated initially
  - IISAS (Viet & Jan) - agreed to provide old GPUs (3 NVIDIA K20) but only for testing purposes, non through VA. Needs registration to the **`vo.access.egi.eu`**
  - INFN CNAF – agreed to provide (through VA) access to (at least) one NVIDIA A100 GPU.
- **Enable federated identity management using one of the available AAI solutions**
  - Discussion ongoing with the use-case on the VO name: decided to use "**vo.amber-sars-cov2.eu**"





Thank you!

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Website: **www.egi.eu/projects/egi-ace**

EGI Foundation

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