Final research report
EOSC short-term grant
Project “BioDynaMo agent-based simulations for COVID-19”

Introduction

This project was carried out under the CERN against COVID-19 taskforce (cern.ch/against-covid-19) initiative.
The technical level of CERN equipment and the high qualification of researchers in the field of modeling allows for a high-quality simulation of the spread of viral particles in closed spaces.
Evaluation of the risk of infection transmission between people in the same space under different conditions (number of people, duration of presence, space configurations) is critically important in contemporary COVID-19 pandemic conditions and allows one to assess the risks of infection with close contacts in workplaces, schools, and public transport.
We developed a new model and computational tools for high-quality airflow modelling based on BioDynaMo and OpenLB, simulating multiple agents’ displacement and aerosol and droplets spreading. We have been working closely together with the researchers from the Division of the Infectious Diseases and Mathematical Modelling, Institute of Global Health of the University of Geneva to make sure that our simulations reflect correctly the many observed cases of virus outbreaks in closed spaces.
Available models do not simulate simultaneously the movement of people, turbulence of airflows and trajectory of viral particles. Many studies are focusing on detailed simulation of droplet/aerosol spreading, but with either fully static individuals, or with mobile single individuals. Some studies simulated agent movement alongside virus spreading but using only a simplistic diffusion mechanism. Thus, simulating multiple agents’ displacement alongside detailed virus particles spreading is a new and relevant contribution to this area of research.

1. Goal and tasks

The goal of the project was modelling the virus (SARS-nCov2) spreading in closed spaces of different configurations with moving people. We wanted to investigate the risk of COVID-19 spreading:

- in different types of confined spaces, with and without ventilation
- with different duration of exposure
- in the context of various activities (movements etc)
- with and without wearing masks

We have split the overall goal into subtasks:

Part 1. Simulation of agents’ displacement in closed spaces (space types: room/auditorium, shop/supermarket, public transport).

Part 2. Modelling aerosol/droplets diffusion and settling (while breathing, talking, coughing). Tracing the airflow and calculating the virus particle concentration.

Part 3. Simulating the turbulence: simulation of airflow and turbulence as the result of people movement and ventilation flows.

Part 4. Calibration and validation: fitting the parameters according to the statistical data and documented virus spreading cases.

2. Methods

To perform the described tasks, we needed to use several modelling systems and programs and to create the interface for data transfer between them (Fig. 1).

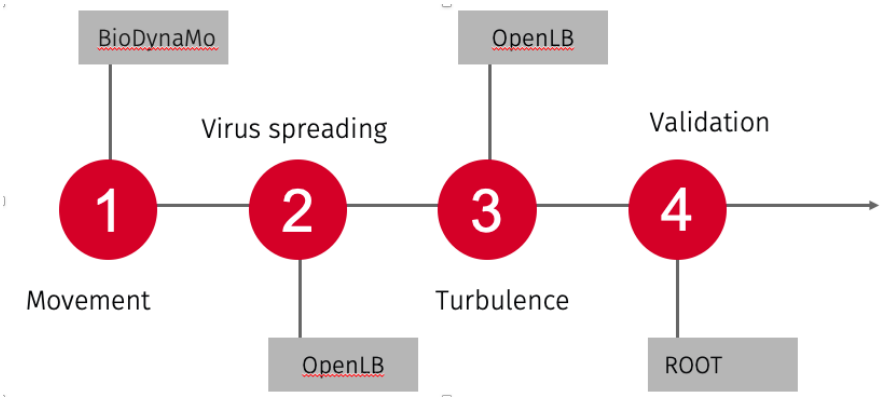

Fig.1. Modelling tasks and simulation packages.

Thus, we have used the agent-based simulation framework BioDynaMo (https://biodynamo.org/) and the Lattice Boltzmann fluid dynamic simulation framework OpenLB (https://www.openlb.net/). The ROOT (https://root.cern.ch/) framework is also used as part of BioDynaMo, and we benefit from the ROOT geometry package (https://root.cern/doc/master/classTGeoManager.html), a tool designed to build detailed geometries and to navigate and query these geometries. These three frameworks are open source and developed in C++, allowing us to use and modify them freely, but also to easily build interfaces between them.

In our simulation framework, we use the ROOT geometry package to precisely construct and describe the environment the simulation will take place in. The geometry package allows the users to easily build different environments and thus implement various simulation scenarios with a high spatial resolution. Several geometries have been constructed, such as a bus and a supermarket. Illustrations of geometries that were constructed with the ROOT geometry package can be found in Fig. 2.

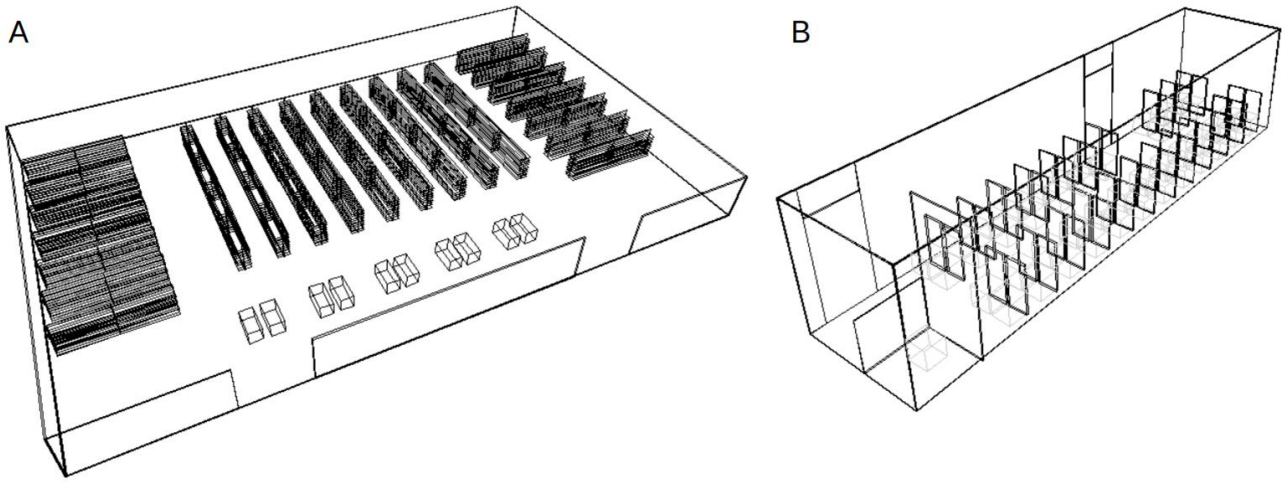

Fig. 2: Simulation environments constructed using the ROOT geometry package, representing a supermarket (A) and a bus (B).

This geometrical description of the environment can then be used by the agent-based simulation framework BioDynaMo.
Here, BioDynaMo is in charge of maintaining and updating all agent characteristics, including their position, orientation and health status (infectious, infected or healthy).

3. Simulation description

We simulate various types of public spaces: classroom, supermarket, bus. For each agent we provide:

- navigation/paths,
- predetermined status (sick, healthy),
- pattern of actions (breathing, talking, coughing, sneezing).

In all scenarios, and at defined intervals of time, the current state of simulation (environment's geometry, agents' position, orientation and health status) is used to initiate a droplet and aerosol spreading simulation.

3.1. Agents' displacement

All agents are physically described as a sphere of 25cm, representing their head. In addition, BioDynaMo simulates agent's behaviours, including the navigation within the environment. The A* algorithm is used in order to calculate the path to follow for an individual to move from one place to another, for instance from the front entrance of the bus to an empty seat. Several navigation behaviours are implemented for each scenario. For instance, in the bus scenario agents can enter the bus through the front door, search for an empty seat, and exit the bus through the rear door. Bus stops are simulated at specified time steps, allowing new agents to enter the bus, and existing agents to leave.
Likewise, in the supermarket scenario, individuals can navigate from one point to another, either following a specified list of destinations, or by randomly choosing destinations. Individuals can enter and exit the building through the entrance door, resulting in the creation and removal of agents in the simulation. These new individuals can be either healthy or contagious.
New scenarios can easily be implemented, building the environment with the ROOT geometry and specifying the behaviour of agents using BioDynaMo. Considered scenarios include a classroom, an open space office and other public transports (airplane, train, metro).

3.2. Virus spreading and turbulence modelling

Using information form the BioDynaMo simulation state, each infectious agent spreads the virus by breathing or coughing. This step is done every five seconds in our simulations but can be tuned by the user. This virus spreading simulation is achieved using the Lattice Boltzmann fluid dynamic simulation framework OpenLB.
Although the epidemic theory distinguishes between droplets and aerosols (Table 1), with the detailed physical modeling we do, considering turbulence and gravity, all particles can be modeled as droplets. Due to their physical properties, the smallest particles form an aerosol that remains in the air for a long time (about two hours), and large droplets move in the air along a parabolic trajectory and settle much faster.

Table 1: Droplets/aerosol virus transmission

DROPLETS	AEROSOL
>5 µm, <100 µm Evaporation: 3s for >50 µm, average <30s. Spread radius: Large droplets (>100 µm) will fall to the floor within a horizontal distance of 2 m from the source (ballistic trajectory).	<5 µm About 80-90% of particles from human respiration <1 µm. Small particles remain airborne for indefinite periods (unless removed due via air currents or dilution ventilation). Spreading radius: 7-8m – sneeze, 2-4.5m – cough.

We simulate the droplets/aerosol spreading considering the distributed size, velocity, and evaporation of the droplets. Droplets are physically represented as interacting particles moved by the airflow and gravity. Airflow turbulences significantly influence the diffusion, and so is explicitly represented through a Smagorinsky turbulence model.
Particles spreading is simulated for five seconds, after which the number of viral particles healthy individuals have been in contact with is transmitted to BioDynaMo.
A particle spreading and air flow simulation using OpenLB is illustrated in Figure 3.

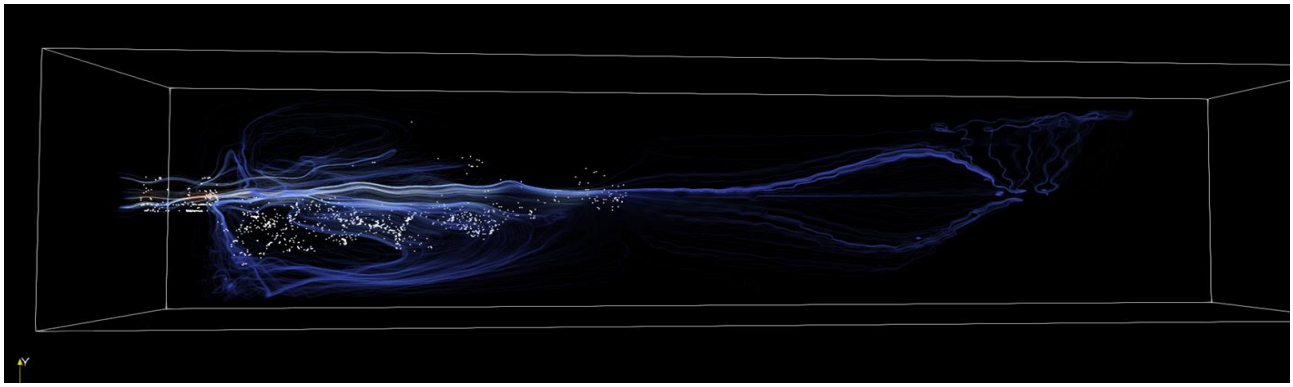

Fig.3. Simulation of particles spreading and air flow using OpenLB in a physical space of 4x4x20m

As fluid dynamic simulations are particularly resource demanding, parallel execution of the program is mandatory. This is achieved using OpenMPI, an open-source implementation of the Message Passing Interface (MPI). Thanks to this, a speed-up of 26x is observed when using 72 cores (divided on 4 NUMA nodes).
In the bus scenario an iteration of the fluid dynamic simulation for 5 seconds takes up to 45 minutes using 72 cores and requires 170 GB of memory. This means that the simulation of 1 minute using our simulation solution requires about nine hours to run (if a five seconds OpenLB simulation occurs every five seconds, 12 OpenLB simulations are needed to simulate one minute).

3.3. Interface between software packages

As BioDynaMo can directly access the data structure containing the ROOT geometry, no specific interface was needed for BioDynaMo to access the geometrical environment information. Typically, a BioDynaMo agent can directly enquiries if a solid structure is nearby, or if a path exists from its location up to a specific point in space.

However, and as MPI does not share memory between processes, an interface is needed between BioDynaMo and OpenLB in order to share agents' characteristics, but also between the ROOT geometry and OpenLB to share the environment geometry. The latter is done by exporting the geometry to a binary STL file, a widely used format in Computer-aided design (CAD) and describing a 3D structure as multiple triangular surfaces. This STL file is then read by OpenLB to initialise and voxelize its 3D environment.
Likewise, the communication between BioDynaMo and OpenLB is done though the export of a file containing information about all agents: position in space, orientation, health status, agent's size and the number of viral particles each agent has been in contact with. This latter information is then updated at the end of the OpenLB simulation and incorporated by BioDynaMo.
A schematic representation of our framework is represented in Figure 4.
In regard to the important runtime needed to complete an OpenLB fluid dynamic simulation, the time needed for read and write operations is negligible.

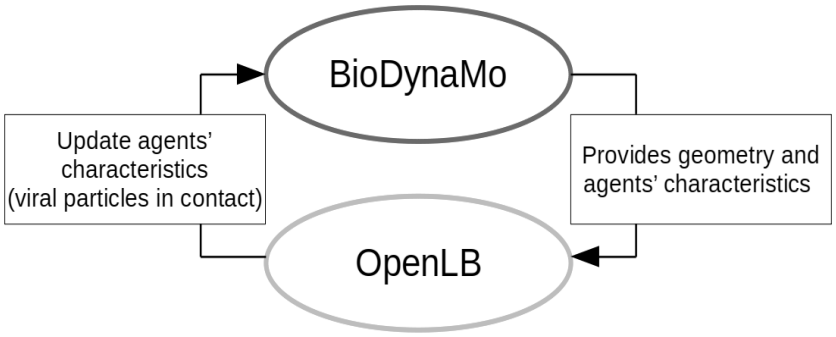

Fig.4. Schematic illustration of the frameworks interface workflow. BioDynaMo is in charge of simulating agent behaviours and characteristics, while the fluid dynamic simulation framework OpenLB is in charge of simulating the precise spreading of droplets and aerosols.

Being simulated independently, the fluid dynamic simulation can be freely modified, or even replaced by another fluid dynamic solver (using for instance a different method than the Lattice Boltzmann one), as long as our input/output format is kept the same.
By this way, additional factors can be considered in this fluid dynamic simulation without impacting the rest of the framework. For instance, it would be possible to add ventilation or convection (transfer of heat due to the movement of a fluid) and thus simulate their effects on the droplets spreading with only a modification of the fluid dynamic part of the simulation.
This is a particularly crucial aspect of our framework, as fluid mechanic simulations are notably resource demanding. Well separated compartments of our framework and a flexible workflow allows the user to adjust and parametrise the fluid dynamic aspect of the simulation as needed.

3.4. Parameters' validation and calibration

Parameters have been calibrated according to real statistical data. This includes the particle sizes distribution, the particle number distribution, viral load of particles (number of viral particles in a droplet) and the infectious dose (number of viral particles an agent must receive to get infected) See table 2.
Importantly, variations are to be noted in data obtained from experiments. For instance, the number of viral particles an individual must receive to have a 50% probability to get infected has been reported to be between ten to one thousand. For this reason, a probabilistic approach has been implemented. Thereby, an individual who received several viral particles during the simulation will only have a small

probability to get infected. Likewise, the number of droplet and aerosol particles expelled by normal breathing follows a gamma distribution with a shape parameter α of 3.5um and a scale parameter β of 2, while the number of particles expelled by a cough follows a gamma distribution with a shape parameter α of 14um with a scale parameter β of 2.6.

Table 2: Simulation parameters (aggregated data from different sources)

	Breathing	Coughing	Sneezing	Speaking
Mean particle size, um	0.3–0.4 (Almstrand, 1989) 0.07 (Holmgren, 2010)	14 (Duguid) 13.5 (Chao et al, 2009)	8.1 (Duguid)	16 (Chao et al)
Gamma distr. GSD	2 (Holmgren, 2010)	2.6 (Duguid)	2.3 (Duguid)	0.55 (Wang, 2020)
Initial velocity (mean) m/s	1 (Xie)	10 (Xie) 11.7 (Chao et al, 2009)	50 (Xie)	3.1-3.9 (Chao et al, 2009)
Virus-laden particles count (mean) copies per 1 act	~650 total particles Rarely any virus-containing ~500 total (Holmgren)	390-2021 (7.00*10^6 - 2.35*10^9 viral load) (Wang, 2020) 947–2085 (Chao et al)		per 1 c: 112–6720 (2.35*10^9 - 1.23 × 10^5 after evaporation viral load) (Wang, 2020) 67.4% of droplets contain viruses

4. Results, applications and extensions

We have developed a new model and set of computational tools for high-quality airflow modelling based on BioDynaMo and OpenLB, simulating multiple agents' displacement and aerosol and droplets spreading.

Using our simulation software, it is possible to take agent dynamics into account instead of simulating only a static snapshot of a situation. This is particularly important to better reflect real world situations especially in cases where many individuals can meet, such as in public transport or shops. This allows us to investigate virus spreading in situations where individuals may only stay in contact during a limited amount of time. By implementing specific scenarios, it is possible to investigate the impact of measures preventing virus spreading, such as social distancing or wearing facial masks. The list of scenarios is represented in the Table 3.

Also, the simulation can be used for calibration and investigating the real-case data about COVID-19 spreading in closed spaces. The possible modelling cases are presented in the Fig. 5.

As already stated, an important benefit of our approach is its flexibility, allowing to easily implement new scenarios (geometry construction, agent behaviour) or to take new mechanisms into account for the fluid mechanic simulation (ventilation, convection, etc.).

Table 3: Possible scenarios

Space	Scenario	Time inside	Distance
Bus/Metro	Agents entering the bus/metro, sitting/standing for a bit, and then leaving	10-60 min	From 0.3–0.5 m
Plane/train	Agents entering the plane, sitting there (mostly motionlessly) during a few hours and then leaving	0.5-5 h	From 1 m
Supermarket	Agents entering the building, walking by the shelves, then leaving	0.5-1 h	Mostly more than 2 m, occasional close interactions
Office	Agents entering the building, sitting at their desk (maybe with short break/lunch) then leaving at the end of the day	8 h	Usually more than 2 m (with sporadic close interactions)
School/class	Agents entering the building, sitting at their desk during the lesson (30 – 90 min), after that go outside and come back in 15-30 min	0.5-1.5 h / break, repeat many times	~1 m, (also exit crowd, interactions while playing together)
Public events (cinema, concerts etc.)	Agents entering the hall, stay there for a few hours, leaving afterwards	2-3 h	1.5-2 m, exit crowd
Elevator	One/few agents inside a low-volume confined space, short-term	1-3 min	0.5 m

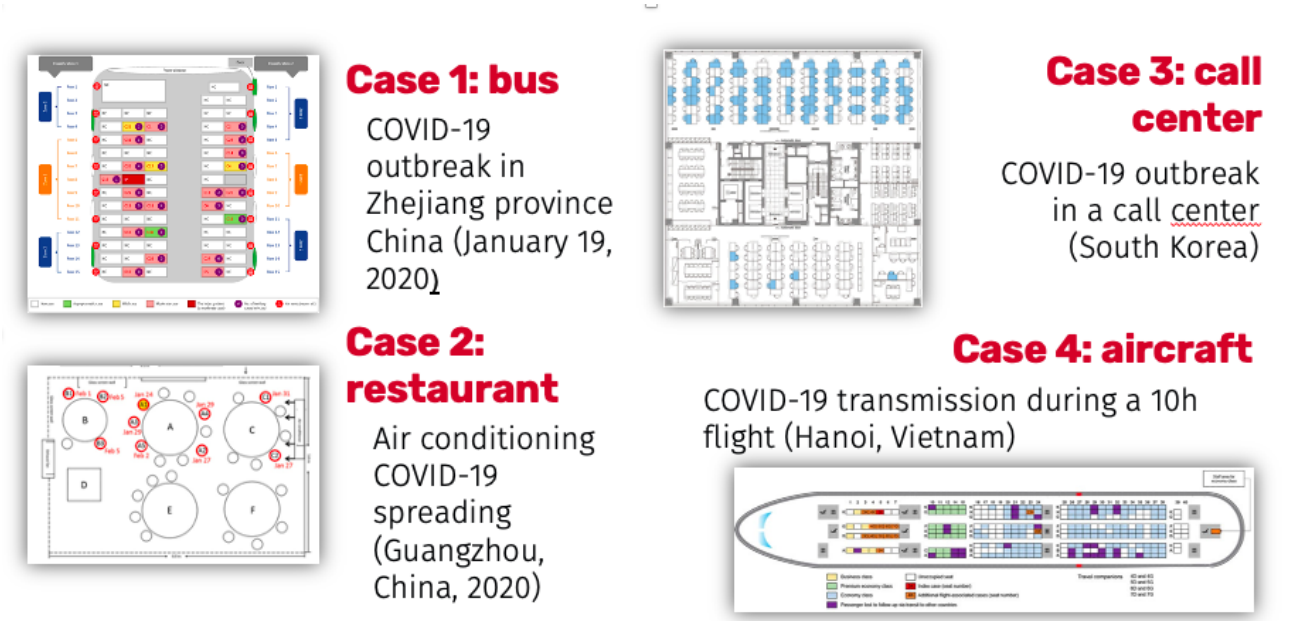

Fig.5. Real-cases outbreak in close space

Acknowledgment

All codes of this project can be found in the following Zenodo online repository: 10.5281/zenodo.5534456
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