Quantifying the Potential of Covid-19 Transmission Across Scales: Using SEM based Navier-Stokes solver to the CEAT

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GOAL: Accurate Prediction of Virus Loading in Indoor Environments

- Currently it is motivated by COVID-19, but the methodology can be used for other respiratory viruses in the future
- Understand the process involved in virus-laden aerosol mixing and transport
- Predict the most probable regions of virus-laden aerosol accumulation and deposition, which will help us to plan

Mitigation Strategies & Compute Risk of Transmission
Modes of Airborne Virus Spreading in the Indoor Environment

• Pre-pandemic, we thought the main mode of airborne transmission of viruses is through coughing and sneezing.

• “Asymptomatic” or “Pre-symptomatic” transmission of Covid-19 has made us question our existing understanding of airborne transmission, especially in the indoor environment.

• If the virus-laden aerosols are helping spread SARS-CoV-2, then it is extremely important understand the spatio-temporal evolution of the aerosols especially in the size range of 0.5 – 20 microns.

Evidence of Long-Distance Droplet Transmission of SARS-CoV-2 by Direct Air Flow in a Restaurant in Korea

Fig. 3. Schematic diagram of the outbreak restaurant equipped with ceiling-type air conditioners. The arrowed solid streamlines represent the air flow directions in the restaurant. Curved air streamlines represent that air streams from the ceiling air conditioners are reflected from the wall or barrier, and move downward toward the floor.
Size of Virus-Laden Aerosol Cloud and what mode will it be transmitted

Isosurface of vertical velocity zones that are high enough to keep 5 micron or lower, aerosols in suspension
If we are using Computational Fluid Dynamics, what level of fidelity is required to accurately capture the aerosol transport?

While each turbulence model has good accuracy in certain flow categories, each flow type favors different turbulence models. Therefore, we summarize both the performance of each particular model in different flows and the best suited turbulence models for each flow category in the conclusions and recommendations.

So we decided to do Direct Numerical Simulation (DNS) or highly-resolution LES, which resolves almost all the relevant scales of turbulence.
First problem we targeted is: DNS of a small cough

\[ w_0(t) = \begin{cases} \frac{w_m}{t_m} t, & 0 \leq t < t_m \\ w_m - \frac{w_m}{t_c-t_m} (t - t_m), & t_m \leq t \leq t_c \\ 0, & t > t_c \end{cases} \]

\[ \begin{align*}
\frac{\partial \tilde{u}_i}{\partial t} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} &= -\frac{\partial \tilde{p}}{\partial \tilde{x}_i} + \frac{1}{Re} \frac{\partial^2 \tilde{u}_i}{\partial \tilde{x}_j \partial \tilde{x}_j} + Ri \tilde{\theta} \delta_{i2}, \\
\frac{\partial \tilde{\theta}}{\partial t} + \tilde{u}_j \frac{\partial \tilde{\theta}}{\partial x_j} &= \frac{1}{Pe} \frac{\partial^2 \tilde{\theta}}{\partial \tilde{x}_j \partial \tilde{x}_j},
\end{align*} \]

\[ Re = \frac{w_m d}{\nu_a} = 6000, \quad Ri = \frac{g \beta_a \Delta T d}{w_m^2} = 5.61 \times 10^{-4} \quad \text{and} \quad Pe = \frac{w_m d}{\alpha_a} = 4200. \]
First problem we targeted is: DNS of a small cough

- Spatial discretization using high-order Spectral Element Methods (SEM) [Nek5000]
- 3rd-order semi-implicit time-stepping, EXT-BDF
- Current simulation has around 300 million computational points, needing 5.2x10^5 CPU hours
- 4, 8, 16, 32, 64, 128 and 256 micron aerosols
- Evaporative and non-Evaporative
  - 200 batches of 69 aerosols
  - ~ 200,000 particles
DNS of a small cough (iso-surface of temperature)
DNS of a small cough
(velocity magnitude [m/s] and temperature [°C] of the cough in space and time)

FIG. 2. Detail of the slice at $x = 0$ of the velocity magnitude field (in m s$^{-1}$) at $t = t_m = 0.15$, 0.25, 0.30, 0.30, 0.75, 1.50 s. Note that $t = t_m = 0.15$ s and $t = t_c = 0.40$ s correspond to the peak and cough ending times respectively.

Previously reported values of $r$ for thermals are 0.25 and between 0.13 and 0.53. In their experiments, Bourouiba, Dehandschoewercker, and Bush found smaller values ranging between 0.09 $\leq r \leq$ 0.18 for the jet stage and 0.015 $\leq r \leq$ 0.037 for the horizontal buoyant phase.

The behavior of a horizontal buoyant puff released with an initial momentum during a short initial period of time ($0 \leq t \leq t_{j,end}$) can be understood as an initial turbulent jet that...
DNS of a small cough
(Puff front evolution and Centroid Location)

Puff front temperature and vertical velocity

Puff centroid location and time
The Dispersed Phase

Non-Evaporating

Evaporating
FIG. 2. Trajectory of particle cloud centroid for evaporative (dashed) and non-evaporative (solid) types. Markers indicate the cough ceasing time for the non-evaporating type. Left panel: 4, 8, 16 and 32 µm. Right panel: 64, 128 and 256 µm. Particles have mostly reached the boundaries of the domain at $r = e_R = 25$. The largest ones, with larger inertia, are the particles that travel the farthest before reaching the bottom domain limits.

On the other side of the particle distribution, particles diameter above 32 µm also exhibit negligible differences in their cloud centroid trajectory. In this case, the shrinking in size due to evaporation over the duration of the experiment is too small to significantly change the particle dynamics dominated, in this case, by the gravitational action.

Notably, evaporation is found to significantly modify the path followed by the 32 µm cloud. While non-evaporative particles follow a parabolic trajectory similar to that described by larger particles, the evaporative cloud counterpart reverses its downward trajectory. This behavior suggests that for this specific size, evaporation leads to a transition from gravity to drag dominated dispersion.
Evaporation

Non-Evaporation

FIG. 2. Caption

FIG. 3. Caption
FIG. 2. Caption

FIG. 3. Caption

Evaporation

Non-Evaporation
Aerosols were injected into the room via a six jet Collison Nebuliser (CN 25, BGI Inc, USA) attached to the inlet port of the chamber. The nebuliser utilises a separate pump, pressure regulator and metre operating at a flow rate of 8 L min$^{-1}$ to deliver HEPA filtered air. Manufacturer's data from BGI indicate the size distribution of particles ejected during the process to have a mean mass diameter of 2.5 μm and a standard deviation of 1.8 μm. Eventual size distribution may vary through evaporation and the experimental set-up. While bioaerosol samples were not taken here, previous studies such as Hathway[4] have shown this experimental approach typically results in a bioaerosol concentration in the room of the order of 10$^3$ to 10$^4$ cfu/m$^3$, with over 90% of the bioaerosols collected on plates 5 and 6 of an Anderson sampler, corresponding to particle diameters of the order 1 μm (Anderson 1958). Method of injection varied based on the requirements for each experimental scenario. In the case of the empty chamber (scenario 1), bioaerosols were released from the centre of the room isotropically. In subsequent cases, (scenarios 2 to 4) a plastic tube of 2.5 cm Ø was clamped at the head of the infectious DIN-man and droplets were released into the thermal plume.

2.3. Sampling methodologies

All biological samples were taken on Tryptone soya agar (Oxoid, UK) as the controlled chamber conditions meant that no other species were present. Deposition was measured using settle plates located on the floor or on surfaces in the room. Given the inherent variability of biological particle collection, it was found that

<table>
<thead>
<tr>
<th>Experimental scenarios</th>
<th>Details</th>
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<tbody>
<tr>
<td>Empty room</td>
<td>No furniture or mannequin</td>
</tr>
<tr>
<td>Single room</td>
<td>Hospital single room &amp; 1 heated mannequin</td>
</tr>
<tr>
<td>Double room</td>
<td>Hospital double room &amp; 2 heated mannequins</td>
</tr>
<tr>
<td>Double room with partition</td>
<td>Hospital double room, 2 heated mannequins &amp; partition between beds.</td>
</tr>
</tbody>
</table>

Aerosol release

| Room centre | Patient head | Patient 1 | Patient 2 | Patient 1 | Patient 2 |

- High-Resolution Large Eddy Simulations (LES) coupled with Lagrangian particle tracking for the aerosols.
- Using high-order Spectral Element Methods for spatial discretization
- Reynolds number: 8000 - 15,000 ~ (4-6-8 ACH)
- Current simulation has 100 million computational points
- 500,000 aerosols (0.5 – 4 -32 microns)
- More expensive, as simulation has to be run longer
Even in a “simple” Empty room the Mixing Process is Complicated
Difference in Dispersion of Aerosols in the Room Based on Location
(a) % Swept Out

(b) Aerosol Diameter (microns)
6 steady-state before 5-micron aerosols were released at four different locations along the center of the room at a height of 1.5-1.7 m.

Figure 2: Figures show the transport of 5 µm aerosols released at four different locations (black squares) driven by airflow at 6 ach, coming in through the vent at the top and going out of the vent at the bottom (red square). Both figures show the velocity magnitude at two planes near the two furthest away walls (colored blue-low flow to red-high flow rates), and demonstrate different pathways the aerosols are transported through depending on their initial location. Notice that the purple particles released in the second from the left black box spread slowly in the center of the room, while the green particles on the far-right black box spread to the right-hand wall.

Figure 3: Figure shows the final distribution (after 360 seconds) of the aerosols starting at four locations when observed through the (a) y-z plane, (b) x-y plane, (c) x-z plane. (d) Percentage of aerosols from each location that were found to go out of the exhaust vent. The green aerosols (P1) that were injected nearest to the wall with the exhaust was found to go out through the vent in the largest numbers. The black aerosols (P4) that were released farthest from the exhaust were the second highest in terms of drain out efficiency.

- Need substantial time to reach a statistical steady state, before aerosols can be injected
- 1.5 mins of real time takes 768 node hours on Frontera (~ 50,000 cpu hours)
- We need to run for at least 30 – 60 mins = 31,000 node hours
- Though it takes about 50,000 node hours to reach a statistically steady state, so each simulation of this size is costing about 100,000 node hours
quantity of infectious material that enters the respiratory tracts of all members of the group by inhalation over the duration of the potential event. Rather than using an explicit calculation of group dose, the CEAT model takes the form of a relative dose model, comparing a specific evaluated scenario to a defined high-risk baseline by a ratio:

\[
\text{Ratio of Group Doses} = \frac{G_i}{G_{BL}}
\]

Fig. 1. CEAT interface and background on the model used. (A) User interface of the interactive PDF for CEAT. (B) The equations (Eqs. 2 to 5) that the CEAT model uses to calculate results. Figures 1A and 1B were created by Jim Gibson of Signature Science, LLC, Charlottesville, Virginia, USA.
The CEAT-predicted infection rate is plotted against the observed cases among the susceptible people (Fig. 2A). Information on vaccination, variant, and mask usage (which was none) was gathered from the reported events (Table 2). The CEAT results show a high correlation with the observed infection rates, with an almost one-to-one relationship (i.e., $R^2 = 0.93$) (Fig. 2A). If we remove case 11 (i.e., Choir rehearsal, France, 12 March 2020) (33, 34) from the data points included, then we achieve an even higher correlation between CEAT and the observed infection rate (i.e., $R^2 = 0.96$). For case 11, CEAT predicted a 100% infection rate, while the actual event had 69% reported infections (Table 2). Given the characteristics of this event, with a reported very small room volume (at 136.5 m$^3$), 27 people singing, and a low ventilation rate, both the CEAT model and the Wells-Riley approach predict a 100% infection rate. As noted in (34), it is possible that cases were underreported; 19 of the 27 individuals reported having COVID-19, including 7 cases confirmed with reverse transcription polymerase chain reaction (RT-PCR) and 12 probable cases that showed symptoms. Because not all individuals were tested with RT-PCR nor directly interviewed by the researcher, we cannot know whether the other assumed that eight negative individuals were asymptomatic and COVID-19 positive or just had unreported symptoms. We believe that including this case shows that although some situations might lack all the optimal parameters needed, CEAT will provide reasonable predictions of the relative magnitude of exposure risk. This is also an argument for testing all individuals in the room in an event such as case 11.
Can we Improve the Computational Performance using GPUs? (NekRS)

- Tests run on 10 nodes of Summit (60 GPUs)
- With a uniform distribution of particles
- **Migration** (Yes/No): Exchanges particle ownership so that each process owns the particles that are present in its elements. (using a fast all-to-all data exchange using *crystal router*).

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<th>CPU</th>
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<td>- Barrier</td>
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Acknowledgments

The research used resources at the Oak Ridge Leadership Computing Facility at Oak Ridge National Laboratory, which is supported by the U.S. Department of Energy, Office of Science and the National Nuclear Security Administration) responsible for the planning and preparation of a capable exascale ecosystem, including software, applications, hardware, advanced system engineering and collaborative e.

Tests run on 10 nodes of Summit (60 GPUs) with a uniform distribution of particles, and the **Migration** (Yes/No): Exchanges particle ownership so that each process owns the particles that are present in its elements. (using a fast all-to-all data exchange using *crystal router*).

Table 1: Cost in iteration on almost every timestep. So, these case is an easy problem for both the particle tracking and the fluid solve. Finally, in the fluid simulation the velocity, pressure, and temperature solves converged within one step. Once at the beginning of the simulation. High particle turnover will produce extra communication distribution will induce load imbalance, which reduces performance. Third, particles were created converge. Second, the particles are distributed uniformly; in many real applications the particle mesh is linear and uniformly sized, meaning that each particle will require migration on their first timestep. So, these case is an easy problem for both the particle tracking and the fluid solve. Finally, in the fluid simulation the velocity, pressure, and temperature solves converged within one step. Once at the beginning of the simulation. High particle turnover will produce extra communication distribution will induce load imbalance, which reduces performance. Third, particles were created converge.

There are a few points to note when extrapolating these results to other cases. First, the particle count will require only one Newton interation to converge. Second, the particles are distributed uniformly; in many real applications the particle mesh is linear and uniformly sized, meaning that each particle will require migration on their first timestep. So, these case is an easy problem for both the particle tracking and the fluid solve. Finally, in the fluid simulation the velocity, pressure, and temperature solves converged within one step. Once at the beginning of the simulation. High particle turnover will produce extra communication distribution will induce load imbalance, which reduces performance. Third, particles were created converge. Second, the particles are distributed uniformly; in many real applications the particle mesh is linear and uniformly sized, meaning that each particle will require migration on their first timestep.
Conclusions and Future Directions from Room-scale Simulations

• We are conducting some of the first high-fidelity turbulence resolved simulations of aerosol transport in indoor environment.

• These simulations will be used as benchmark results to compare/improve lower-fidelity models (e.g. RANS based)

• Improved understanding of effect of aerosol size, release location, air-flow rates and evaporation on residence time and deposition pattern of virus-laden aerosols

• The high-resolution model results are being used to analyze and understand the large and small scale turbulent structure of the flow
Final Objective: Development of a robust Covid-19 Exposure Assessment Tool (CEAT)
Potential Viral Load (based on particle size and concentration) from the Cough

(a) Non-Evaporation

(b) Non-Evaporation
Room scale flow structure at 6 ACH
Evaporation

Non-Evaporation