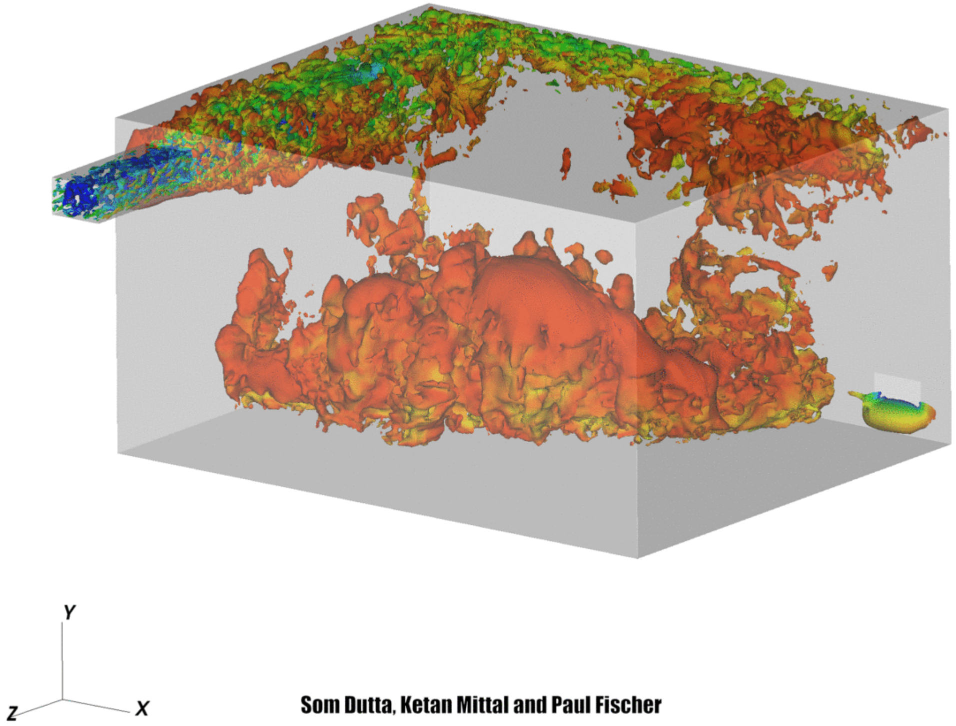
Quantifying the Potential of Covid-19 Transmission Across Scales: Using SEM based Navier-Stokes solver to the CEAT

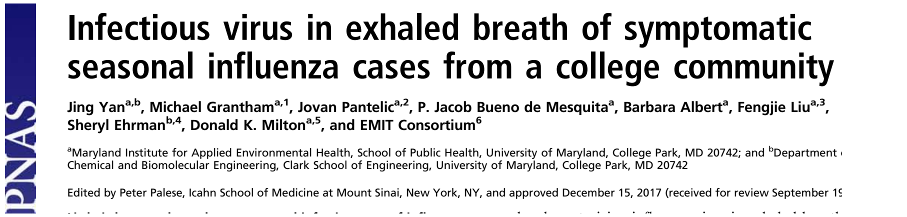
Som Dutta
Mechanical & Aerospace Engineering
Utah State University

Alex Fabregat, Universitat Rovira i Virgili
Jordi Pallares, Universitat Rovira i Virgili
Ketan Mittal, LLNL
K Rao, ANL
Brian J. Schimmoller, Signature Sc. LLC
Afshin Beheshti , NASA & Cov-IRT
Nídia S. Trovão, NIH
Paul Fischer, UIUC
Neil Lindquist,
 Misun Min
Ramesh Balakrishnan, ANL



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


PNAS

Infectious virus in exhaled breath of symptomatic seasonal influenza cases from a college community

Jing Yan[a,b], Michael Grantham[a,1], Jovan Pantelic[a,2], P. Jacob Bueno de Mesquita[a], Barbara Albert[a], Fengjie Liu[a,3], Sheryl Ehrman[b,4], Donald K. Milton[a,5], and EMIT Consortium[6]

[a]Maryland Institute for Applied Environmental Health, School of Public Health, University of Maryland, College Park, MD 20742; and [b]Department
Chemical and Biomolecular Engineering, Clark School of Engineering, University of Maryland, College Park, MD 20742

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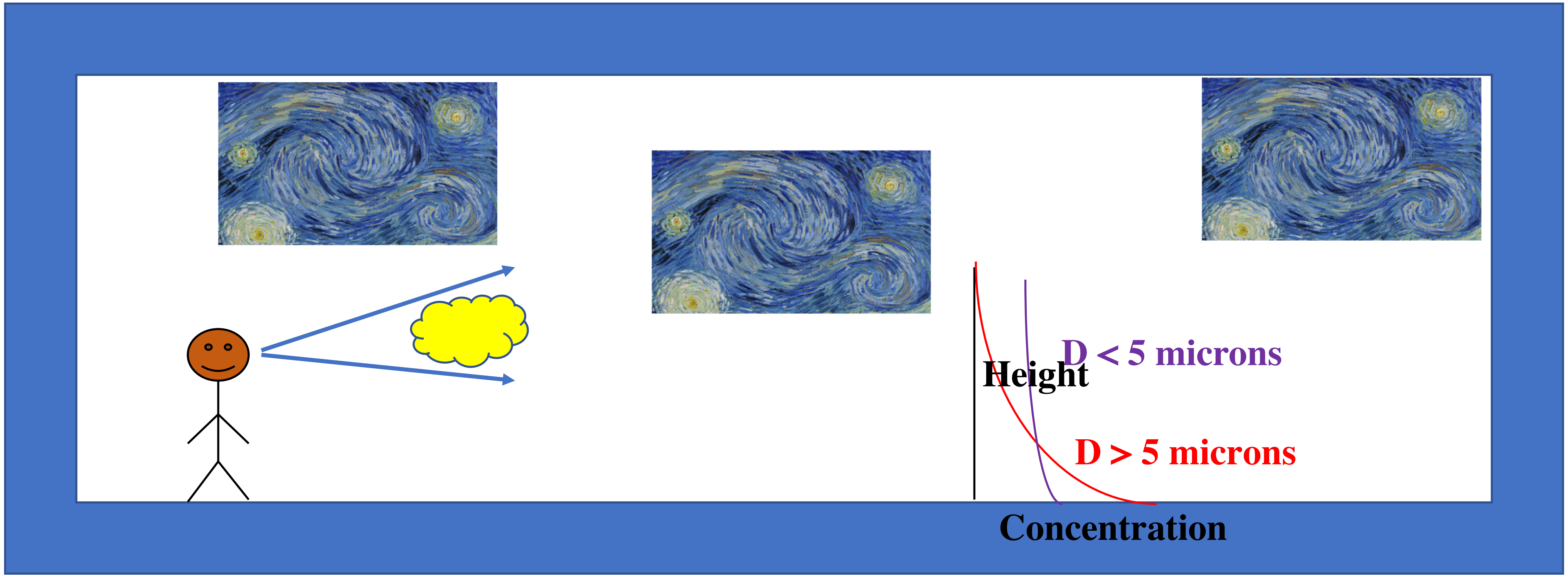
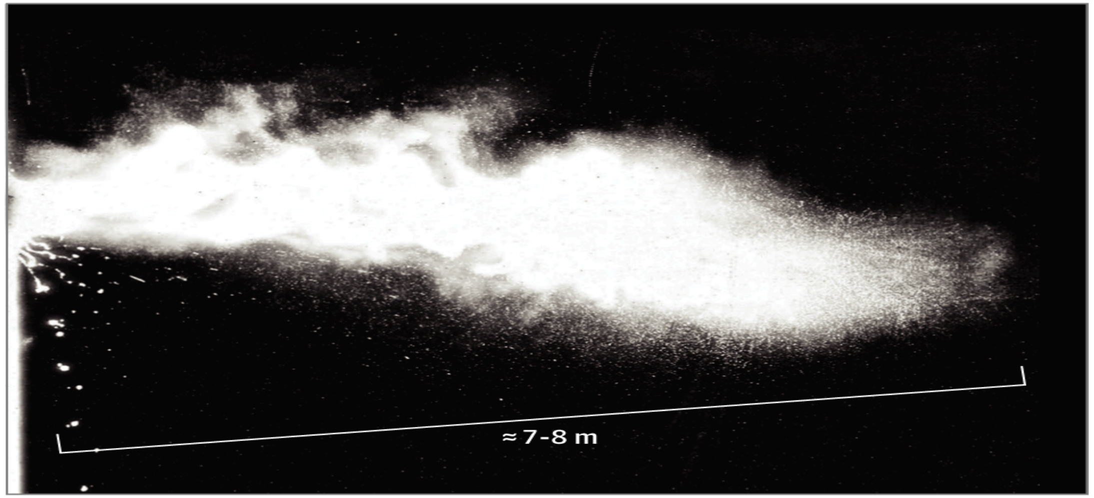


Modes of Airborne Virus Spreading in the Indoor Environment



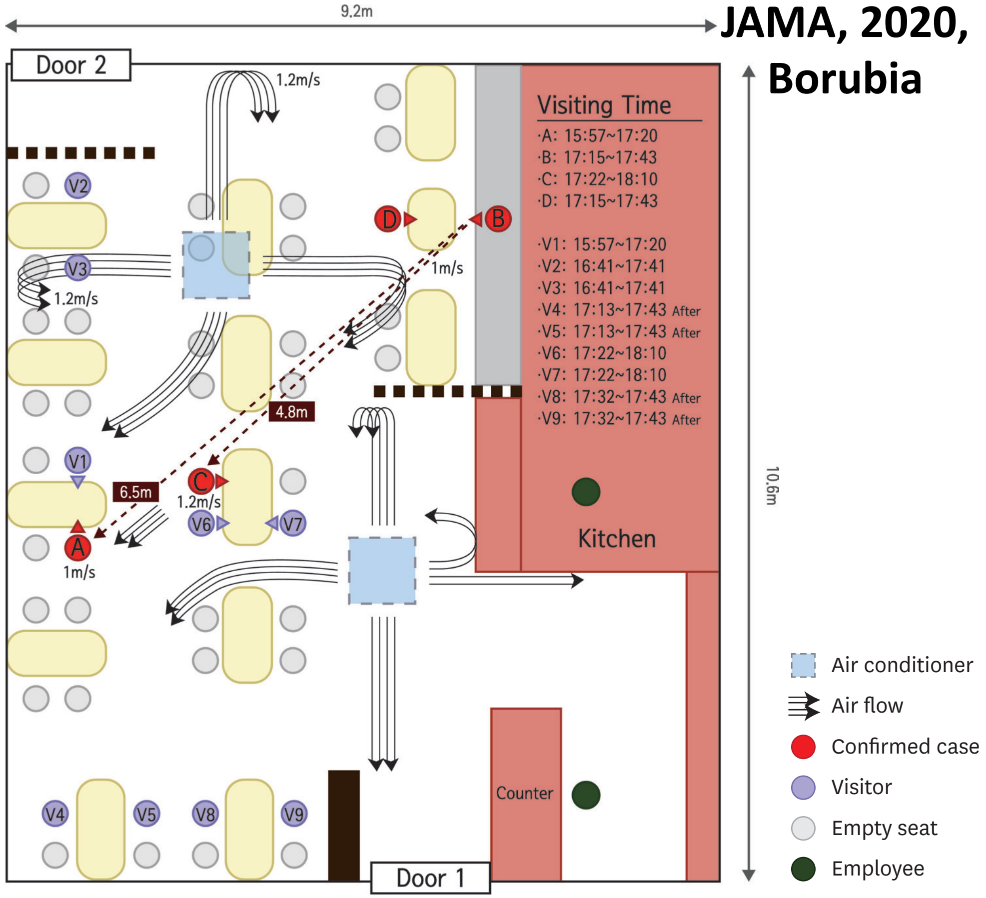
- Pre-pandemic, we thought the main mode of airborne transmission of viruses is through coughing and sneezing

JAMA, 2020, Borubia

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

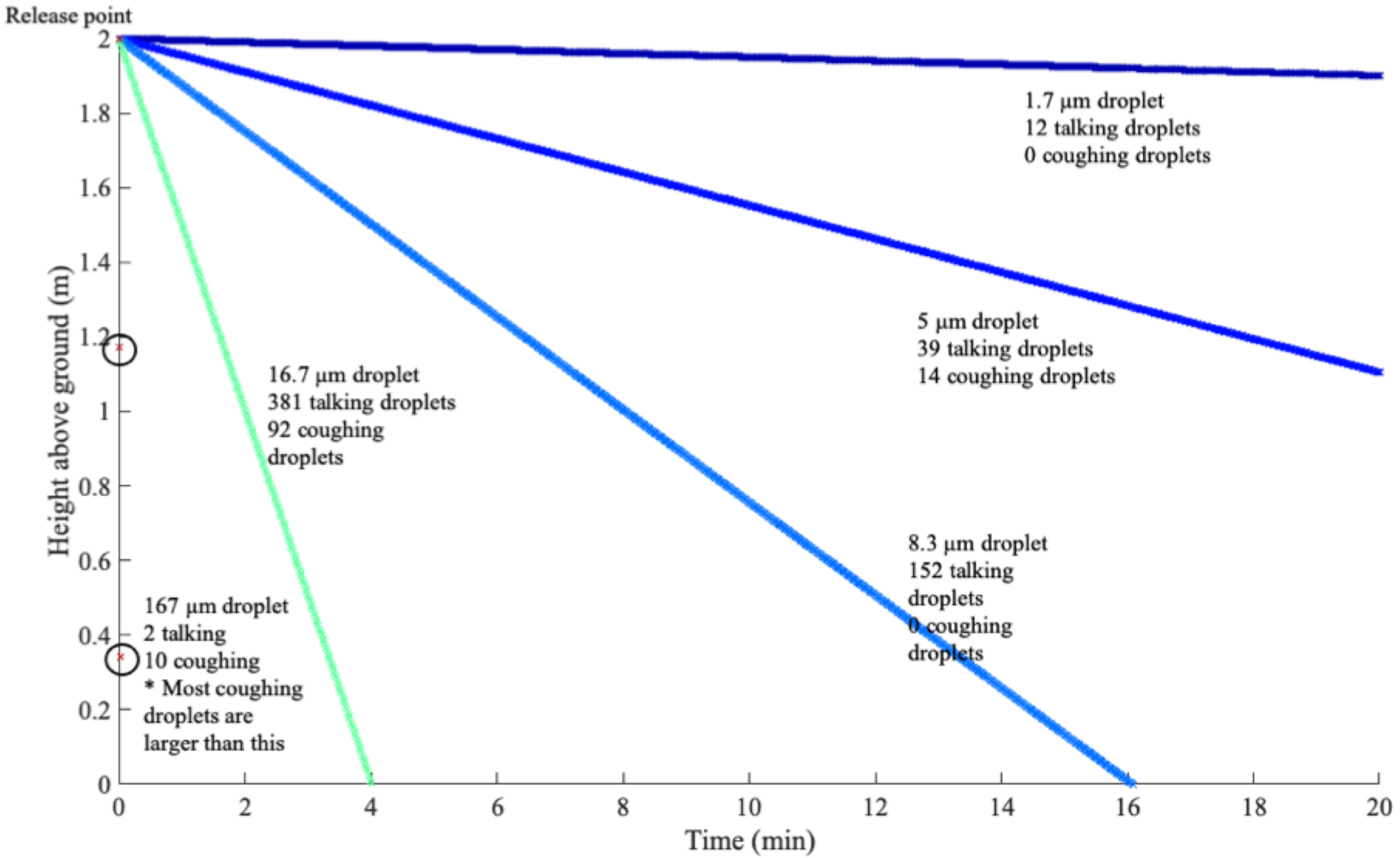
Evidence of Long-Distance Droplet Transmission of SARS-CoV-2 by Direct Air Flow in a Restaurant in Korea

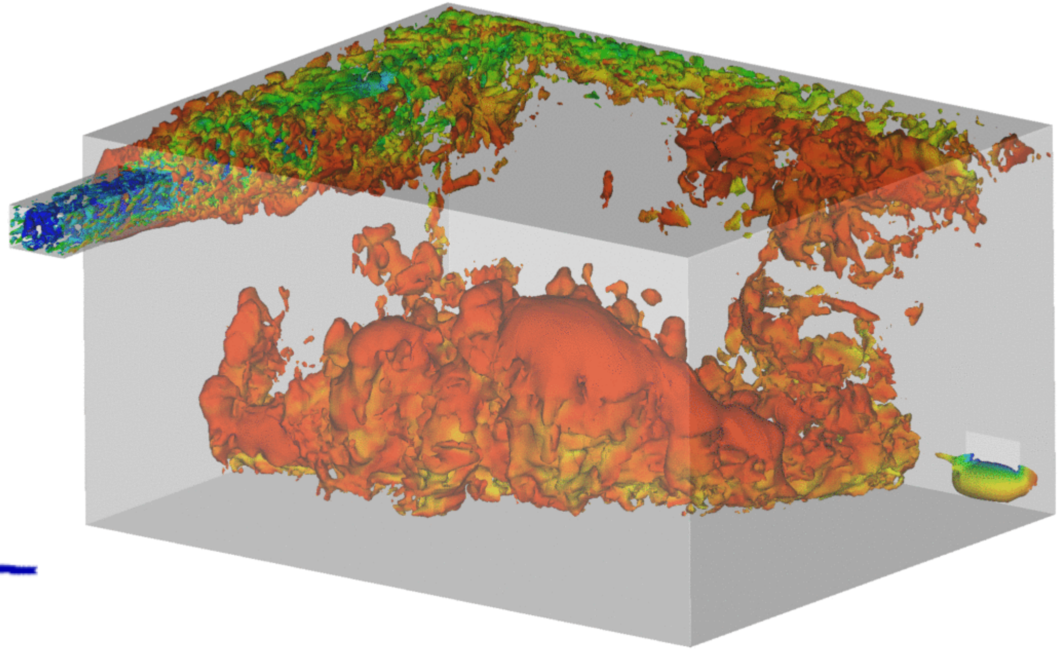
Keun-Sang Kwon [1,2*] Jung-Im Park [2*] Young Joon Park [3] Don-Myung Jung [4] Ki-Wahn Ryu [5] and Ju-Hyung Lee [1,2]



- 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

Size of Virus-Laden Aerosol Cloud and what mode will it be transmitted





Som Dutta, Ketan Mittal and Paul Fischer

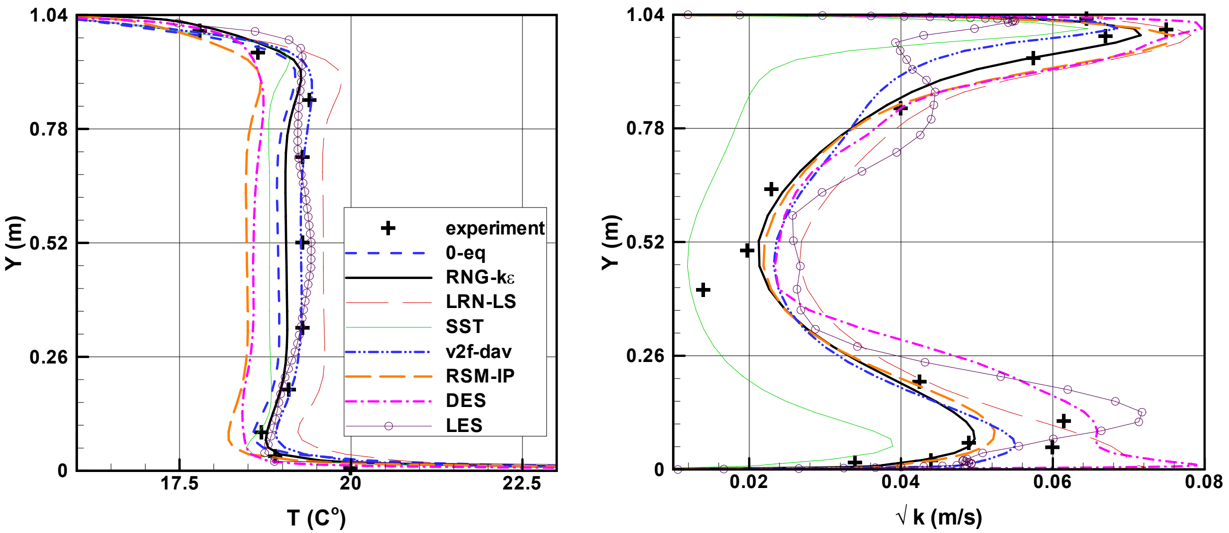
Isosurface of vertical velocity zones that are high enough to keep 5 micron or lower, aerosols in suspension

If we are using Computational Fluid Dynamics, what level of fidelity is required to accurately capture the aerosol transport ?

Evaluation of Various Turbulence Models in Predicting Airflow and Turbulence in Enclosed Environments by CFD: Part-2: Comparison with Experimental Data from Literature

(2007)

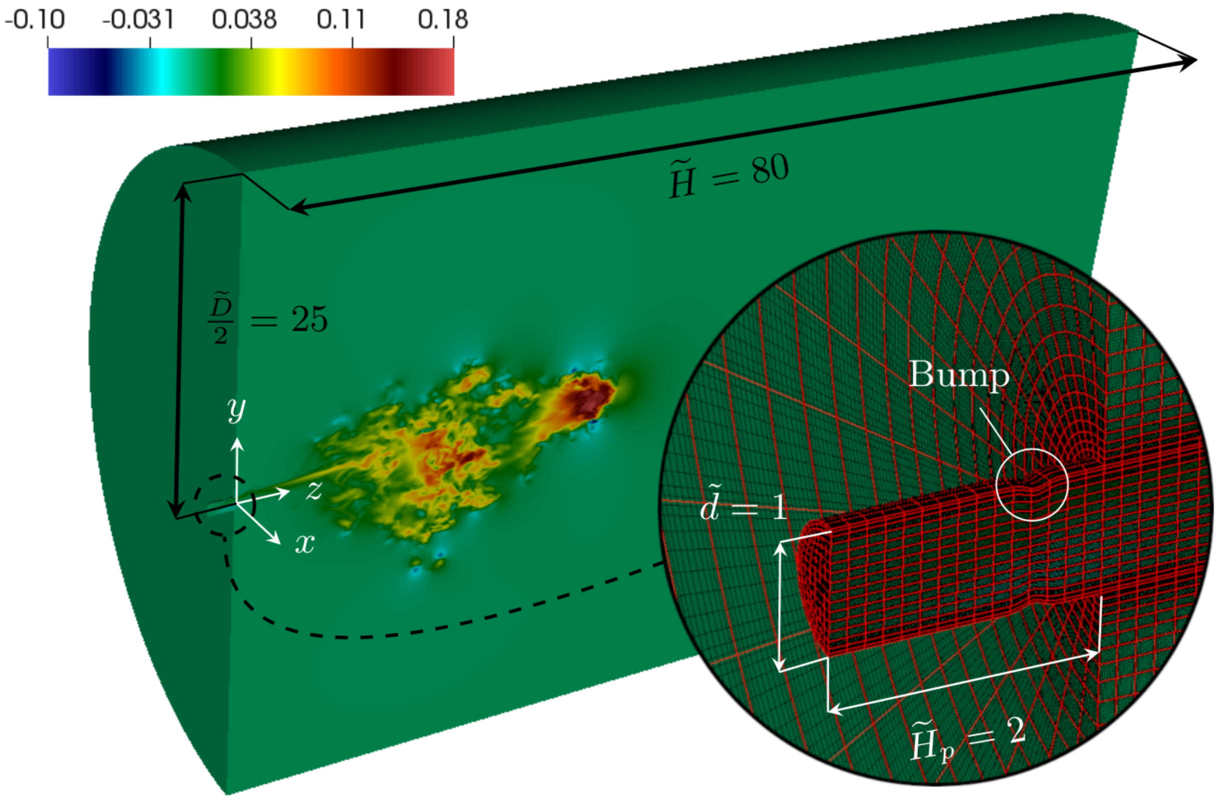
Zhao Zhang, Student Member ASHRAE
Wei Zhang, Member ASHRAE
Zhiqiang Zhai, Member ASHRAE
Qingyan Chen*, Fellow ASHRAE



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 partcular 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



$$w_0(t) = \begin{cases} \frac{w_m}{t_m} t, & 0 \le t < t_m \\ w_m - \frac{w_m}{t_c - t_m}(t - t_m), & t_m \le t \le t_c \\ 0. & t > t_c \end{cases}$$

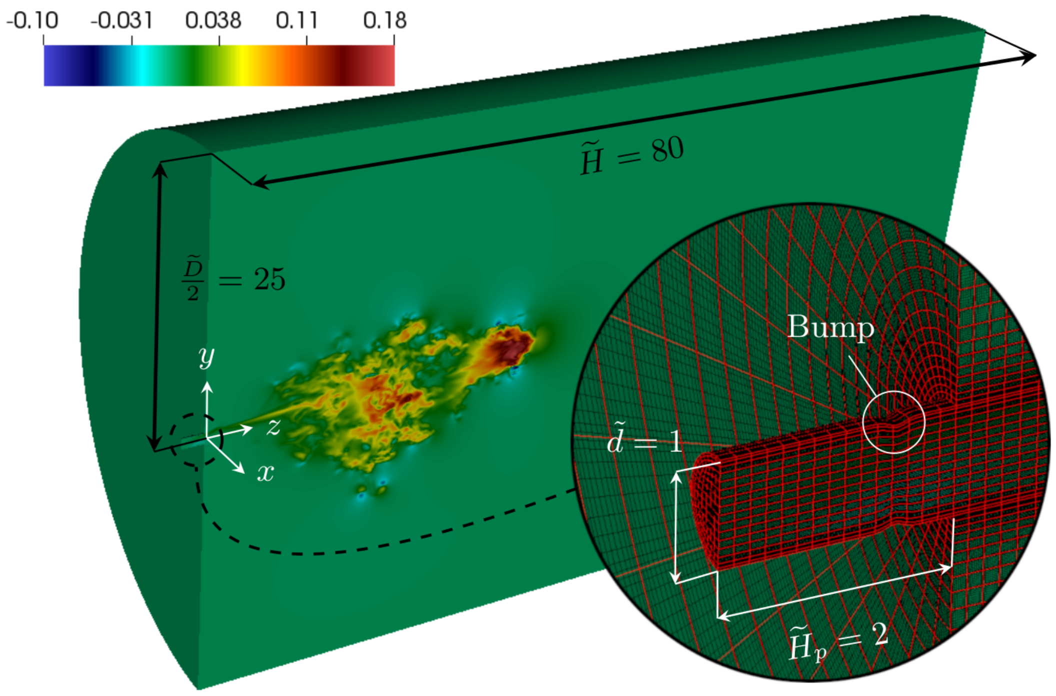
$$\frac{\partial \tilde{u}_i}{\partial \tilde{x}_i} = 0,$$

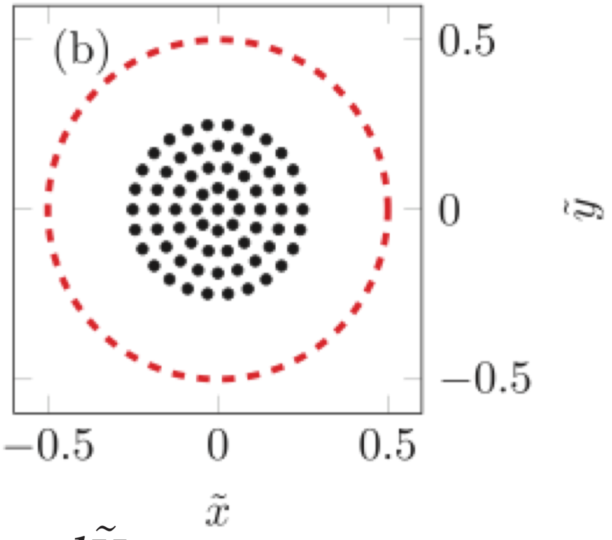
$$\frac{\partial \tilde{u}_i}{\partial \tilde{t}} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial \tilde{x}_j} = -\frac{\partial \tilde{p}}{\partial \tilde{x}_i} + \frac{1}{Re} \frac{\partial^2 \tilde{u}_i}{\partial \tilde{x}_j \partial \tilde{x}_j} + Ri\, \tilde{\theta}\, \delta_{i2},$$

$$\frac{\partial \tilde{\theta}}{\partial \tilde{t}} + \tilde{u}_j \frac{\partial \tilde{\theta}}{\partial \tilde{x}_j} = \frac{1}{Pe} \frac{\partial^2 \tilde{\theta}}{\partial \tilde{x}_j \partial \tilde{x}_j},$$

$Re = w_m d/\nu_a = 6000,\ Ri = g\beta_a \Delta T d/{w_m}^2 = 5.61 \times 10^{-4}$ and $Pe = w_m d/\alpha_a = 4200.$

First problem we targeted is: DNS of a small cough





$$\frac{d\tilde{X}_i}{d\tilde{t}} = \tilde{U}_i,$$

$$\frac{d\tilde{U}_i}{d\tilde{t}} = \underbrace{\frac{\tilde{u}_i - \tilde{U}_i}{\tau_p}}_{\text{Drag}} + \underbrace{n_g \delta_{i2}}_{\text{Buoyancy}} + \underbrace{n_{th} \frac{\partial \tilde{\theta}}{\partial \tilde{x}_i}}_{\text{Thermophoresis}}. \qquad \tau_p = Re \frac{\tilde{d}_p^2}{18 C_c} \frac{\rho_p}{\rho_a} \left(1 + 0.15 Re_p^{0.687}\right)^{-1}$$

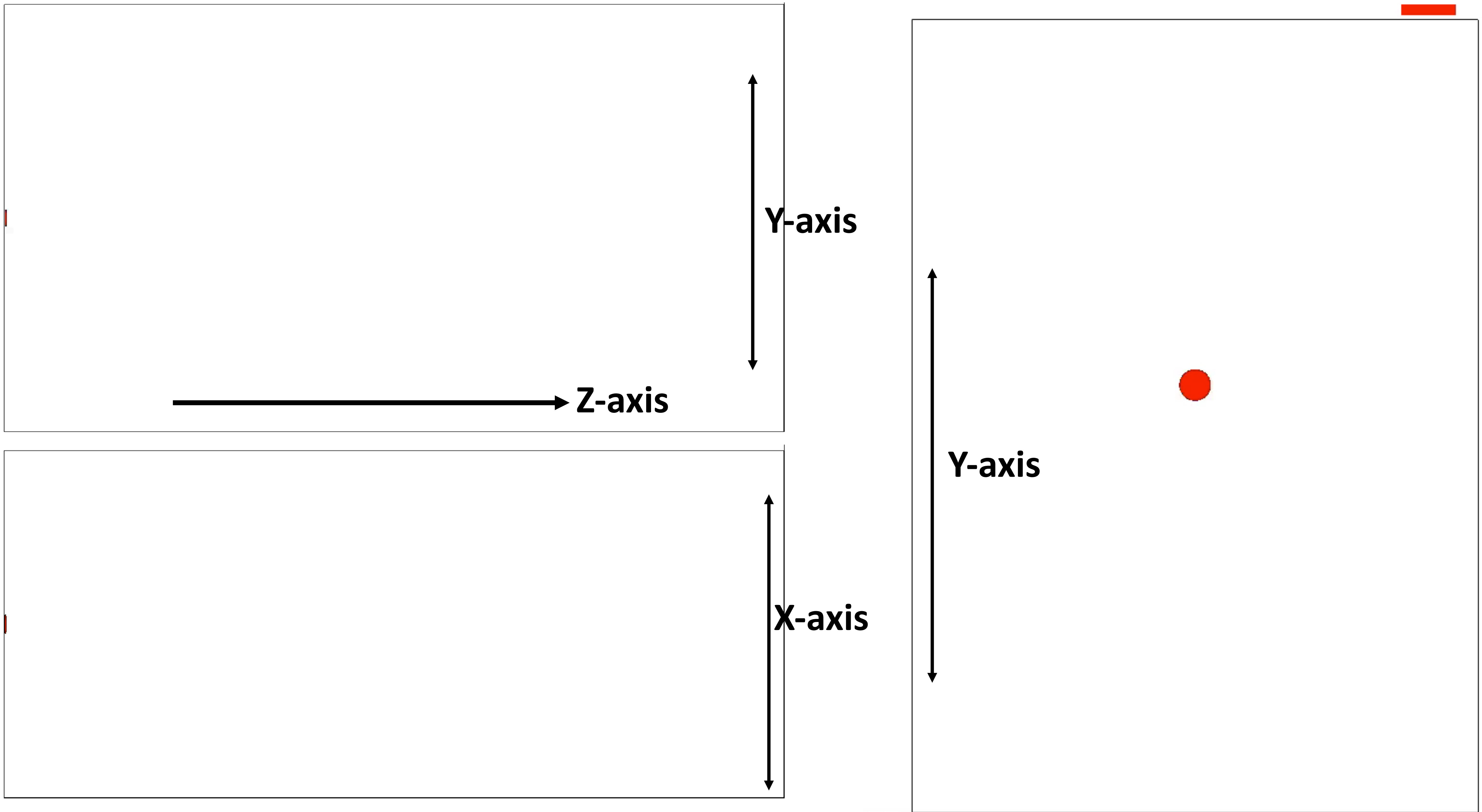
$$\frac{d\,\tilde{d}_p}{d\,\tilde{t}} = \frac{4}{Re\, Sc_v} \frac{\rho_f - \rho_s}{\rho_p} \frac{1}{\tilde{d}_p}, \quad \frac{d\,\tilde{\theta}_p}{d\,\tilde{t}} = \frac{12}{Re\, Pr_p} \frac{1}{\tilde{d}_p^2} \left[\frac{k_v}{k_p} \left(\tilde{\theta}_f - \tilde{\theta}_p \right) + \frac{D_v \Delta H_v}{k_p \Delta T} (\rho_f - \rho_s) \right]$$

- **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 5.2×10^5 CPU hours**

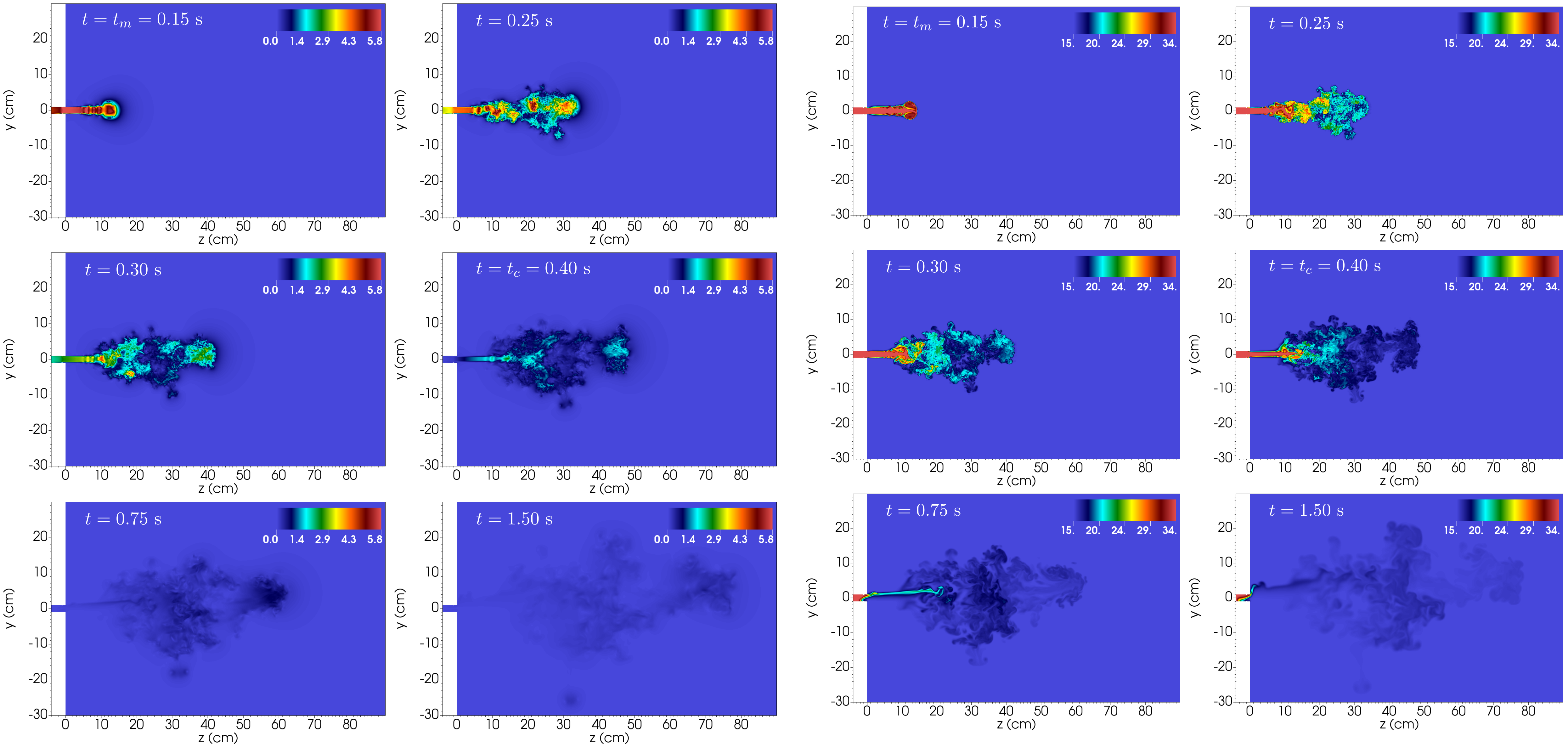
- **4, 8, 16, 32, 64, 128 and 256 micron aerosols**
- **Evaporative and non-Evaporative**
- **200 batches of 69 aerosols**

- **~ 200,000 particles**

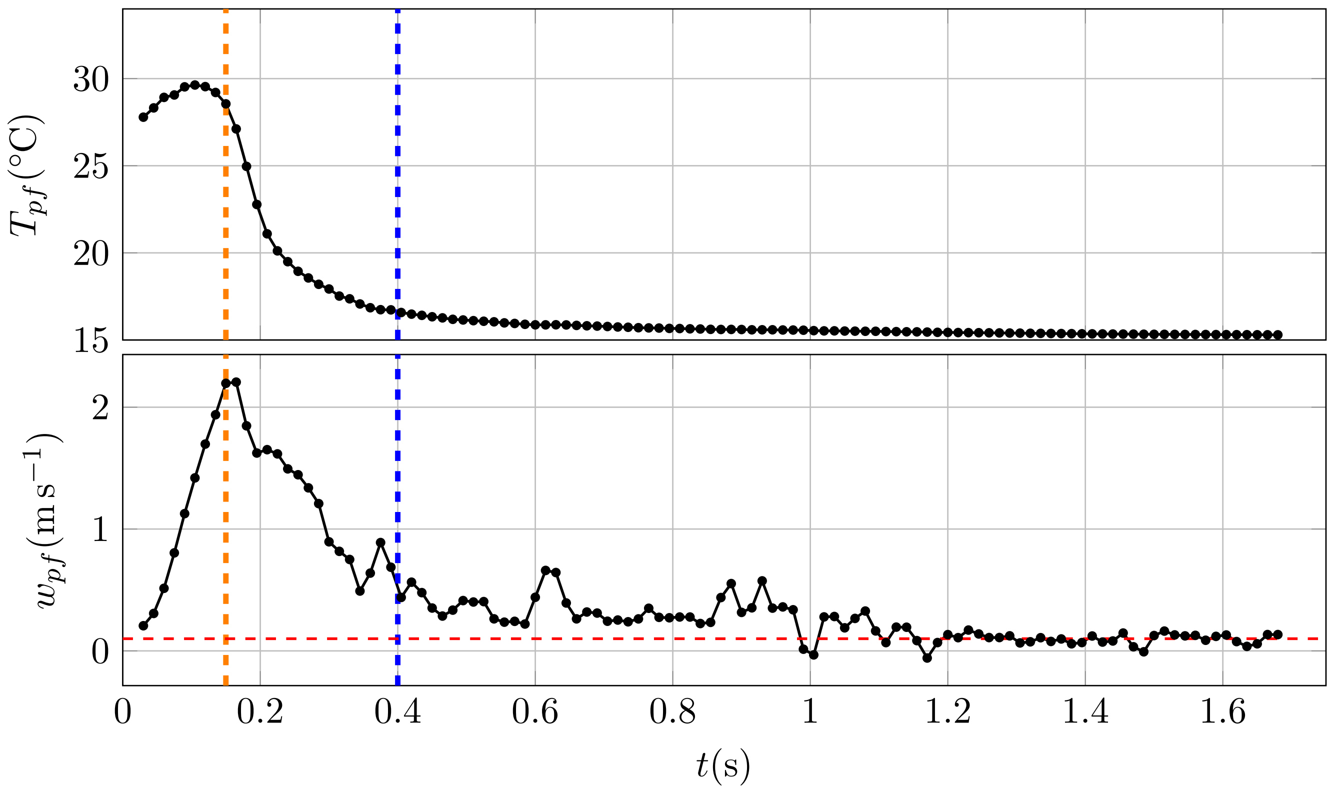
DNS of a small cough (iso-surface of temperature)



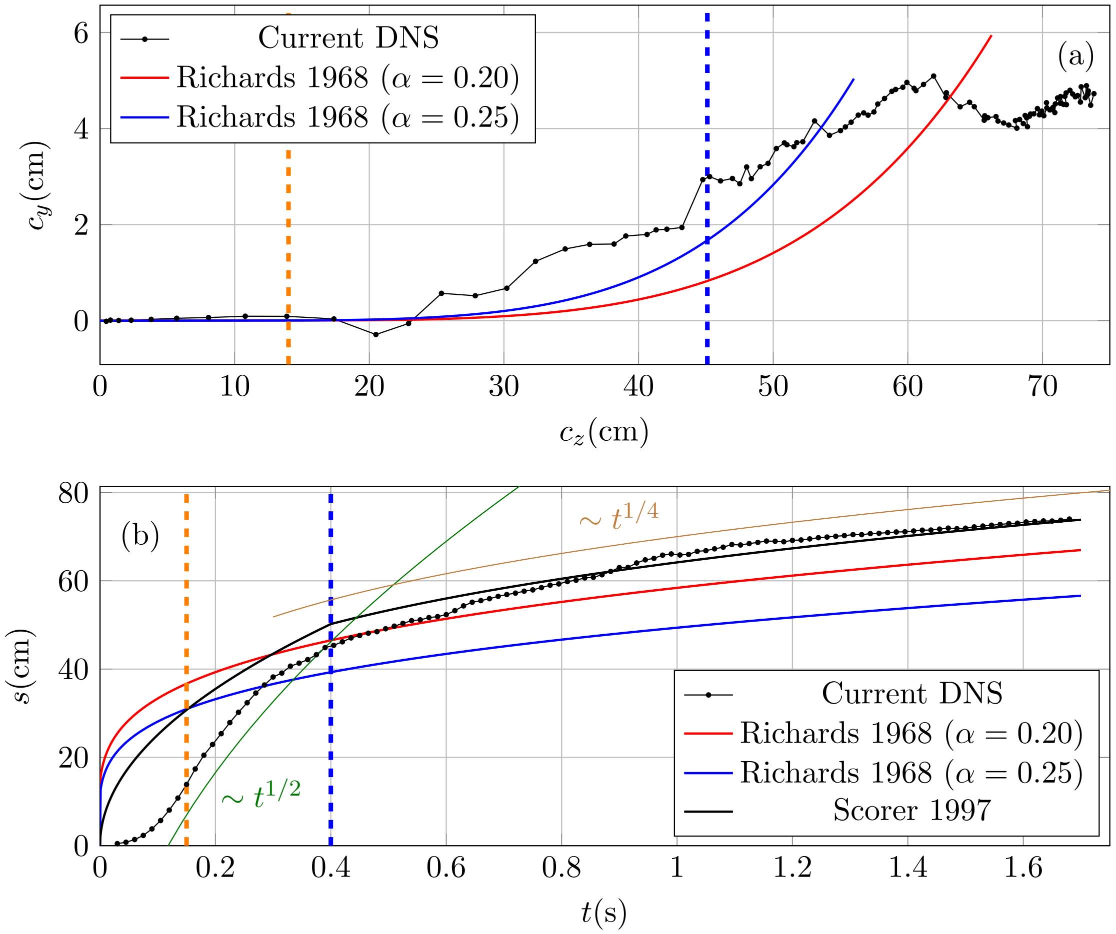
DNS of a small cough
(velocity magnitude [m/s] and temperature [C] of the cough in space and time)



DNS of a small cough
(Puff front evolution and Centroid Location)

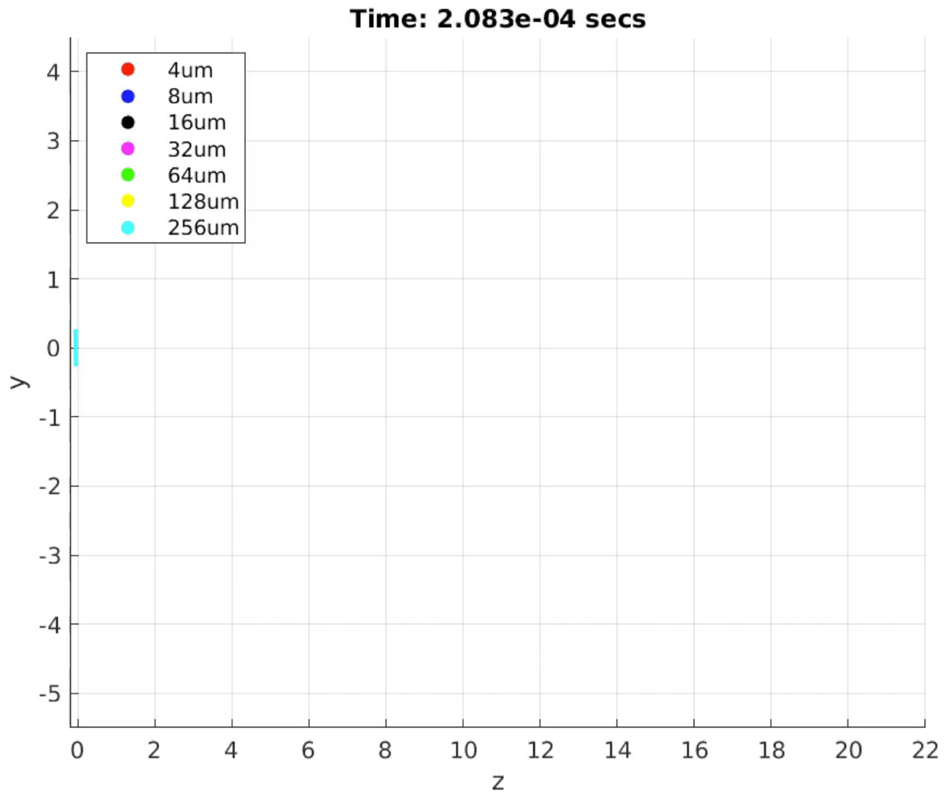


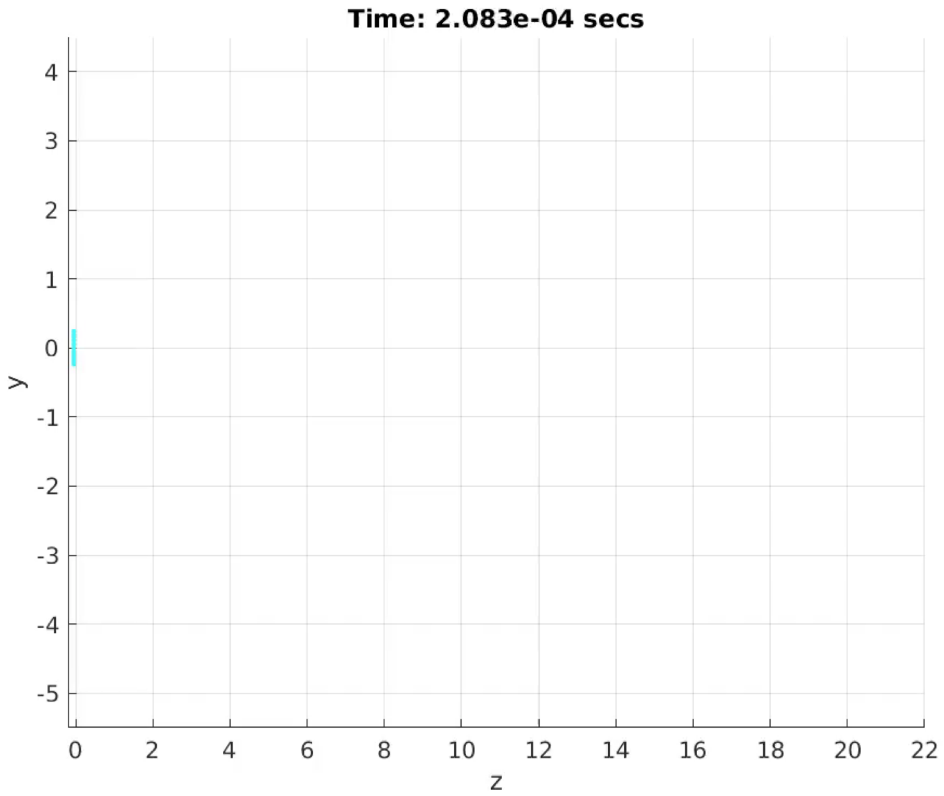
Puff front temperature and vertical velocity



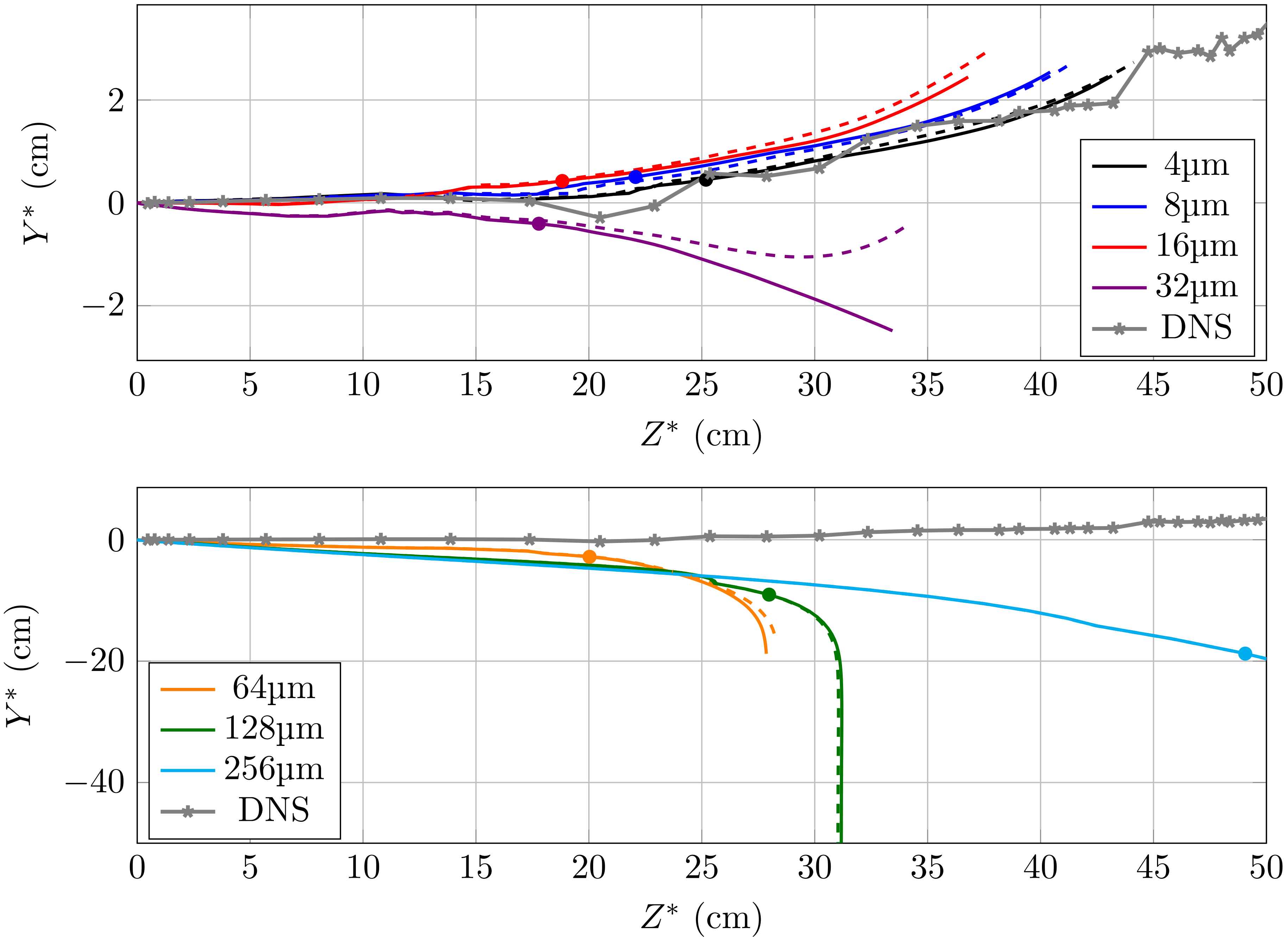
Puff centroid location and time

The Dispersed Phase



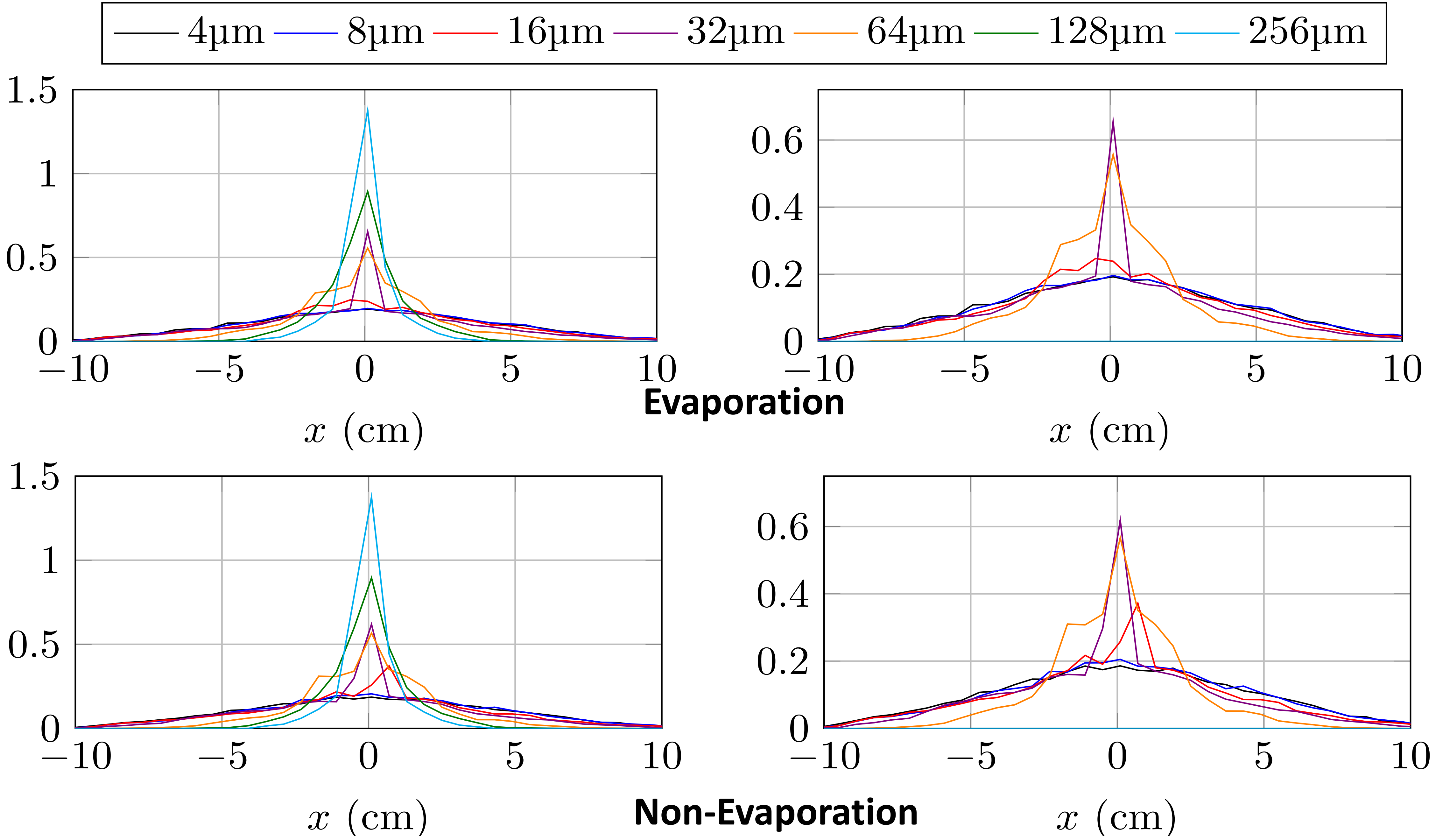


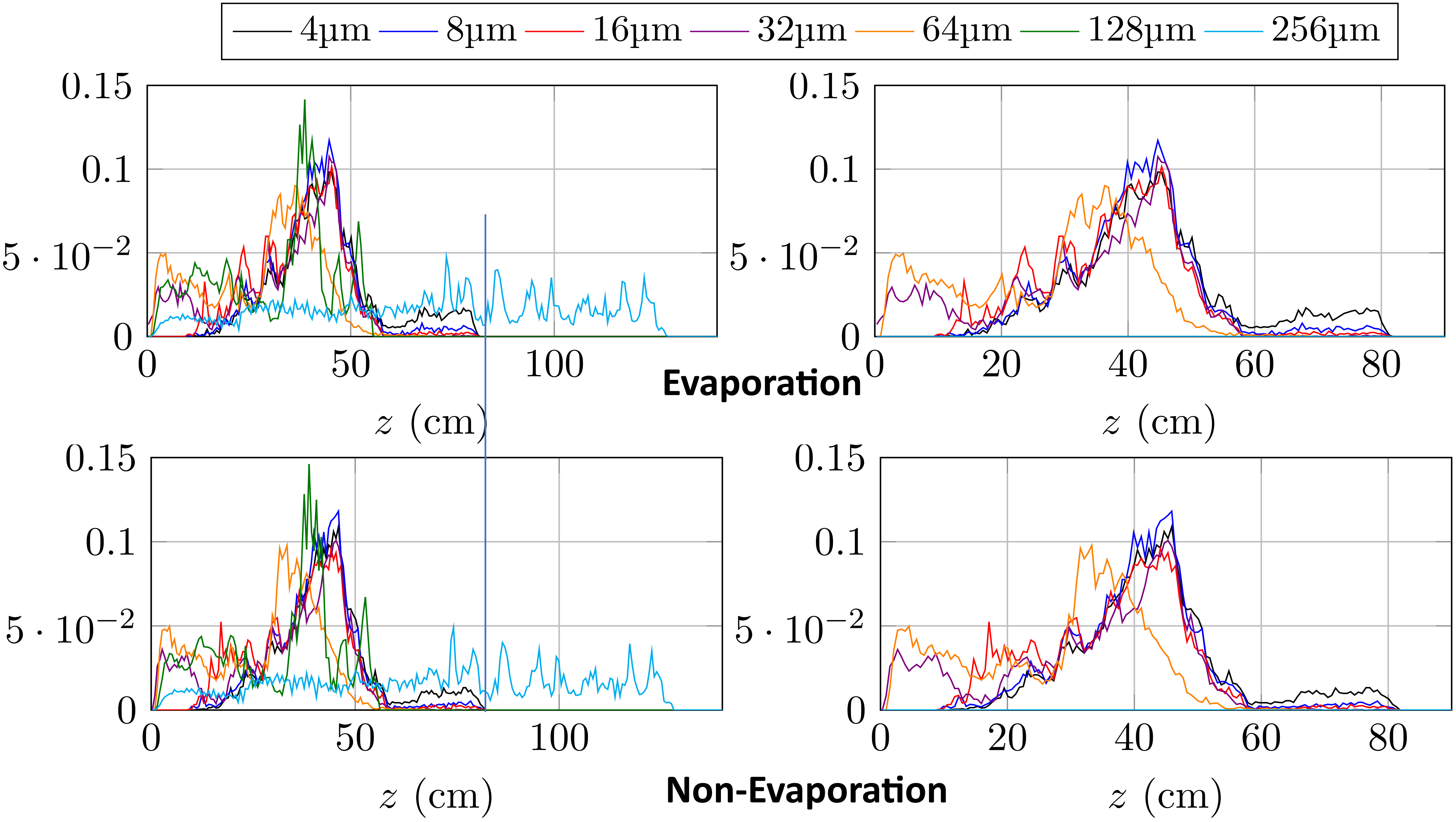
Non-Evaporating **Evaporating**



Dashed – Evaporation

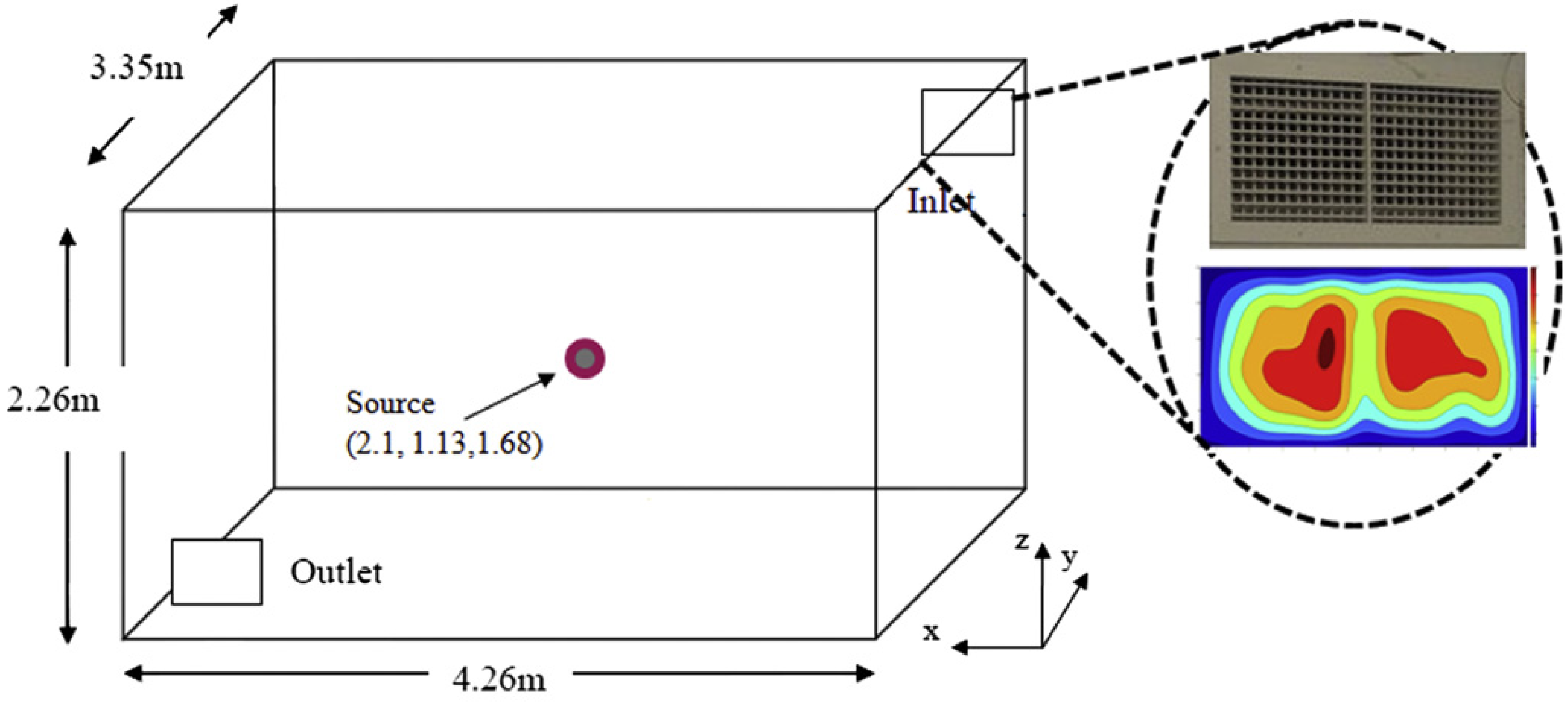
Solid – non-Evaporation


4µm
8µm
16µm
32µm
64µm
128µm
256µm
1.5
1
0.5
0
0.6
0.4
0.2
−10
−5
0
5
10
Evaporation
x (cm)
Non-Evaporation



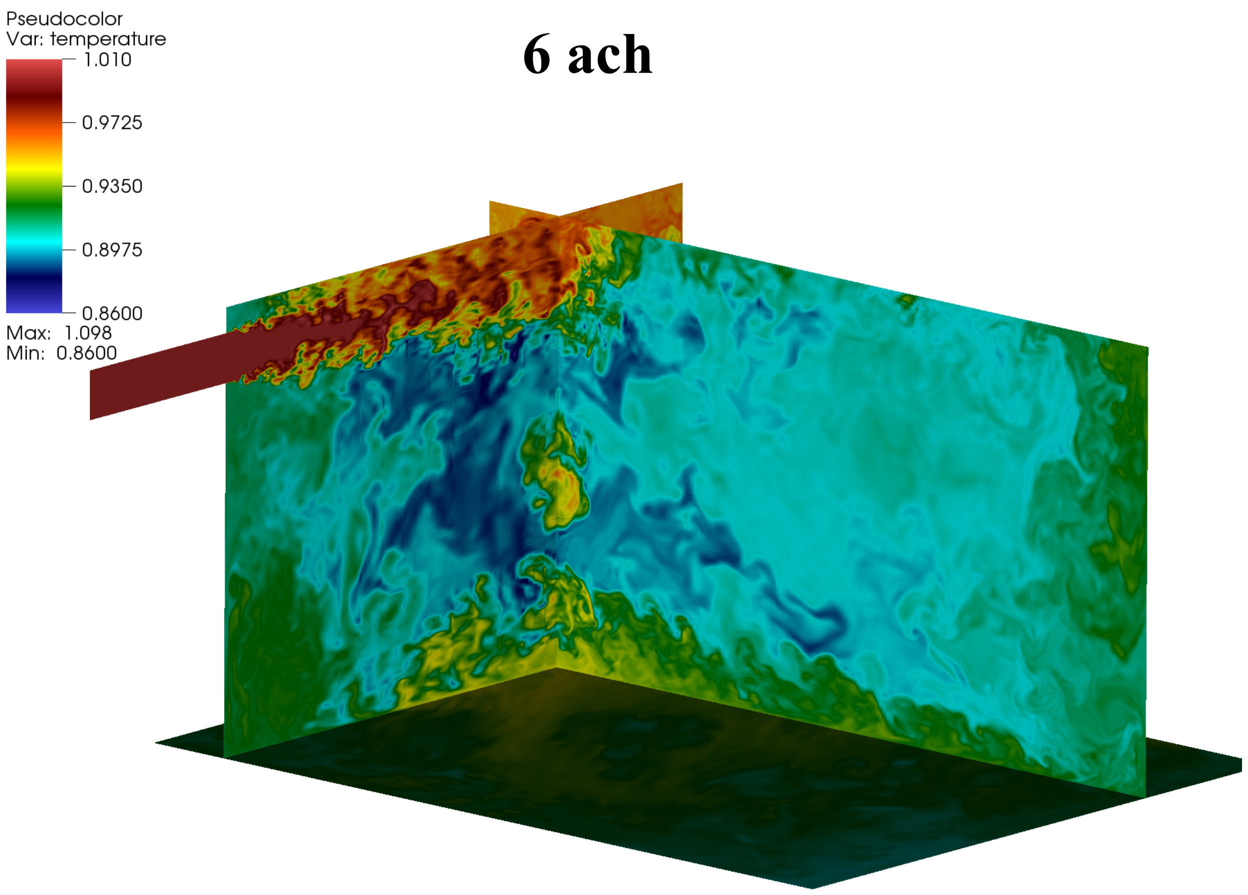
4µm
8µm
16µm
32µm
64µm
128µm
256µm
0.15
0.1
$5 \cdot 10^{-2}$
0
0
50
100
20
40
60
80
z (cm)
Evaporation
Non-Evaporation

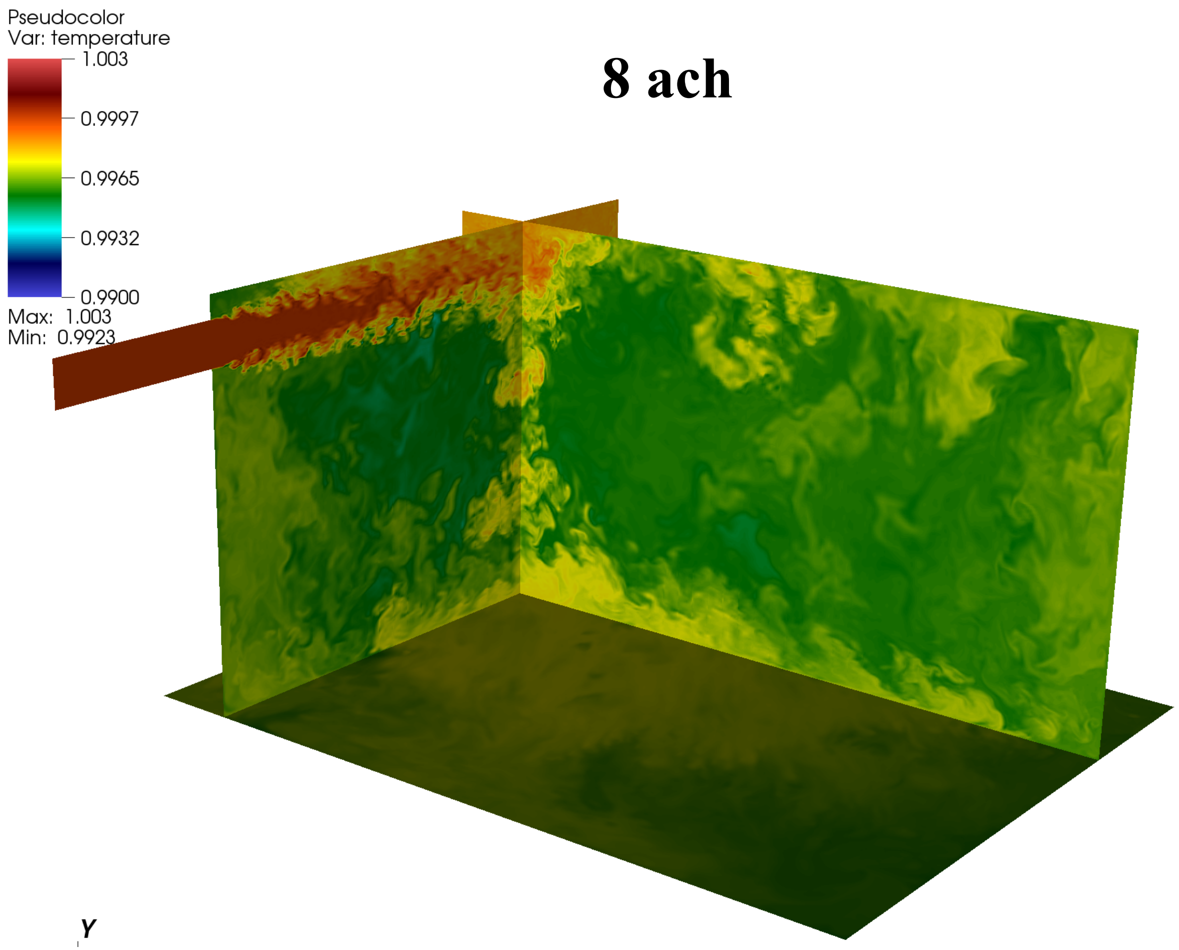
High-Resolution LES of flow and particle transport in a room



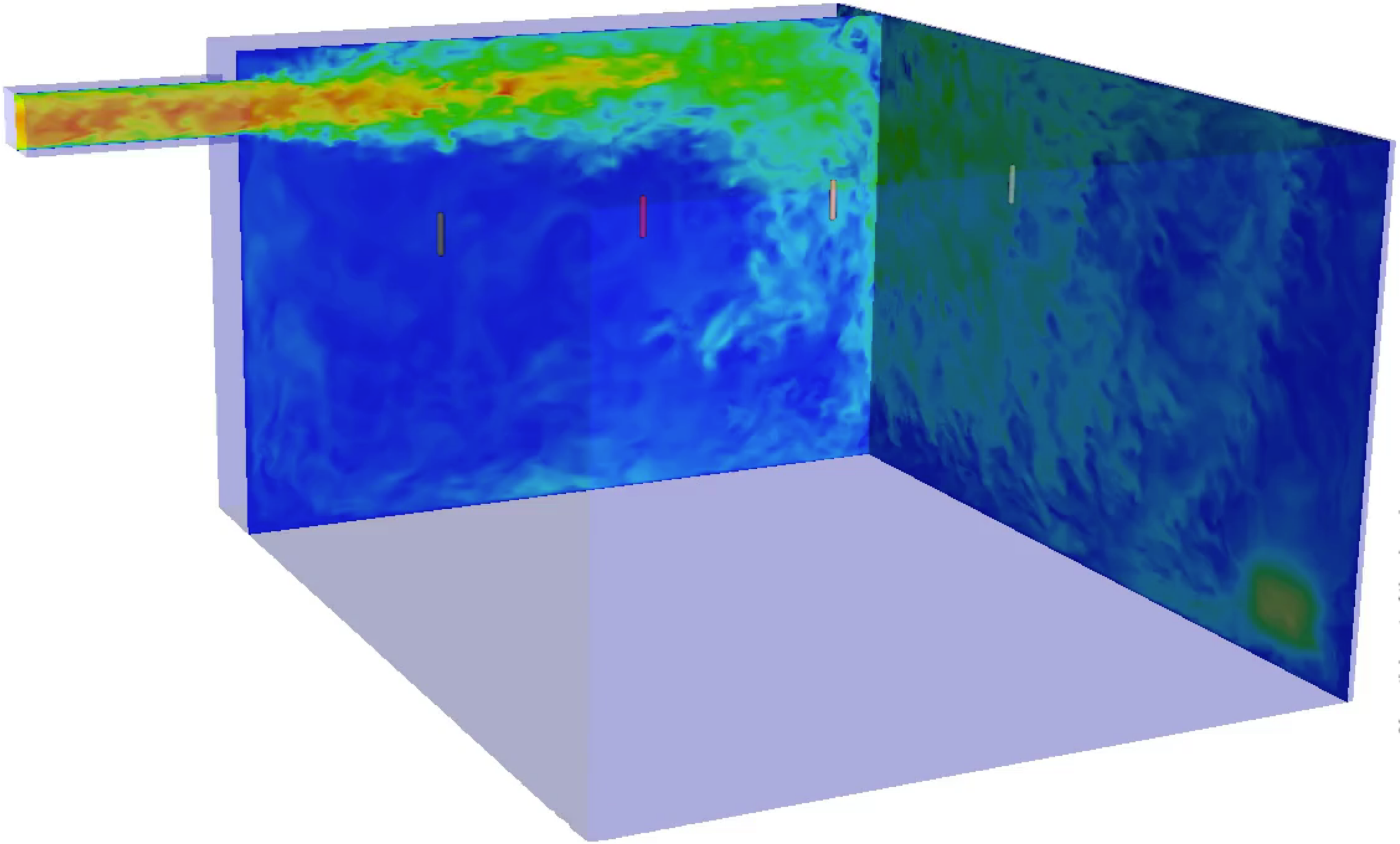
- High-Resolution Large Eddy Simulations (LES) coupled with Lagrangian particle tracking for the aerosols.
- Using high-order Spectral Element Methods for spatial discretization
- Reynolds number: 8000 - 15,000 ~ (4-6-8 ACH)
- Current simulation has 100 million computational points
- 500,000 aerosols (0.5 – 4 -32 microns)
- More expensive, as simulation has to be run longer

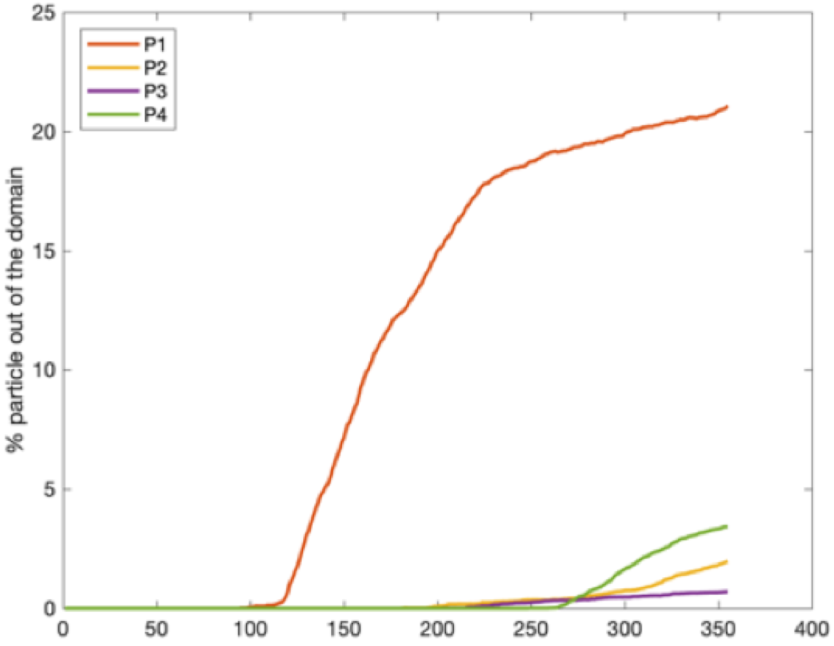
Even in a “simple” Empty room the Mixing Process is Complicated

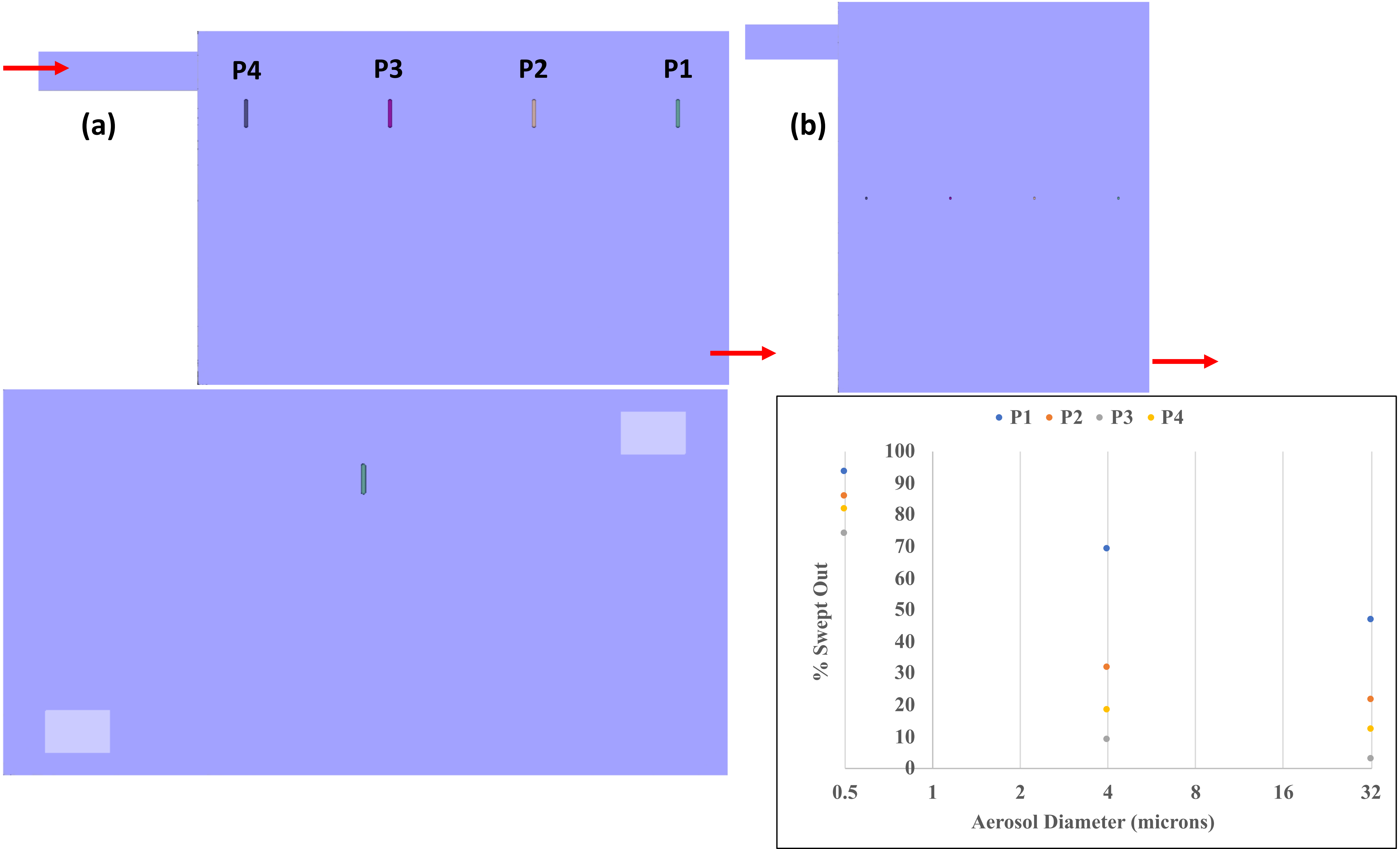




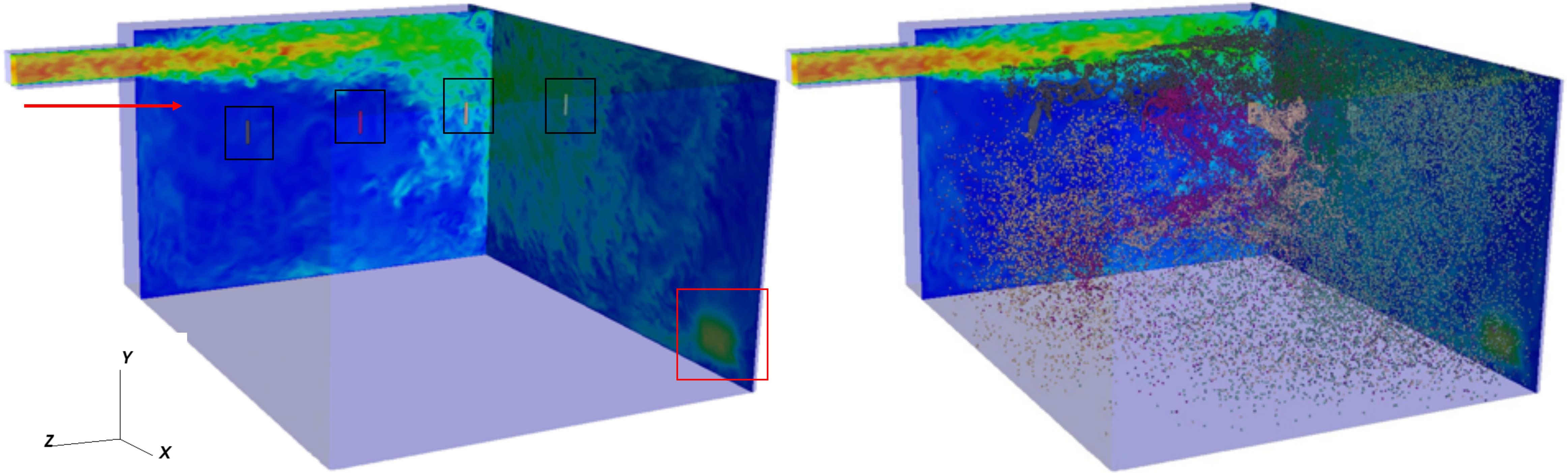
Difference in Dispersion of Aerosols in the Room Based on Location





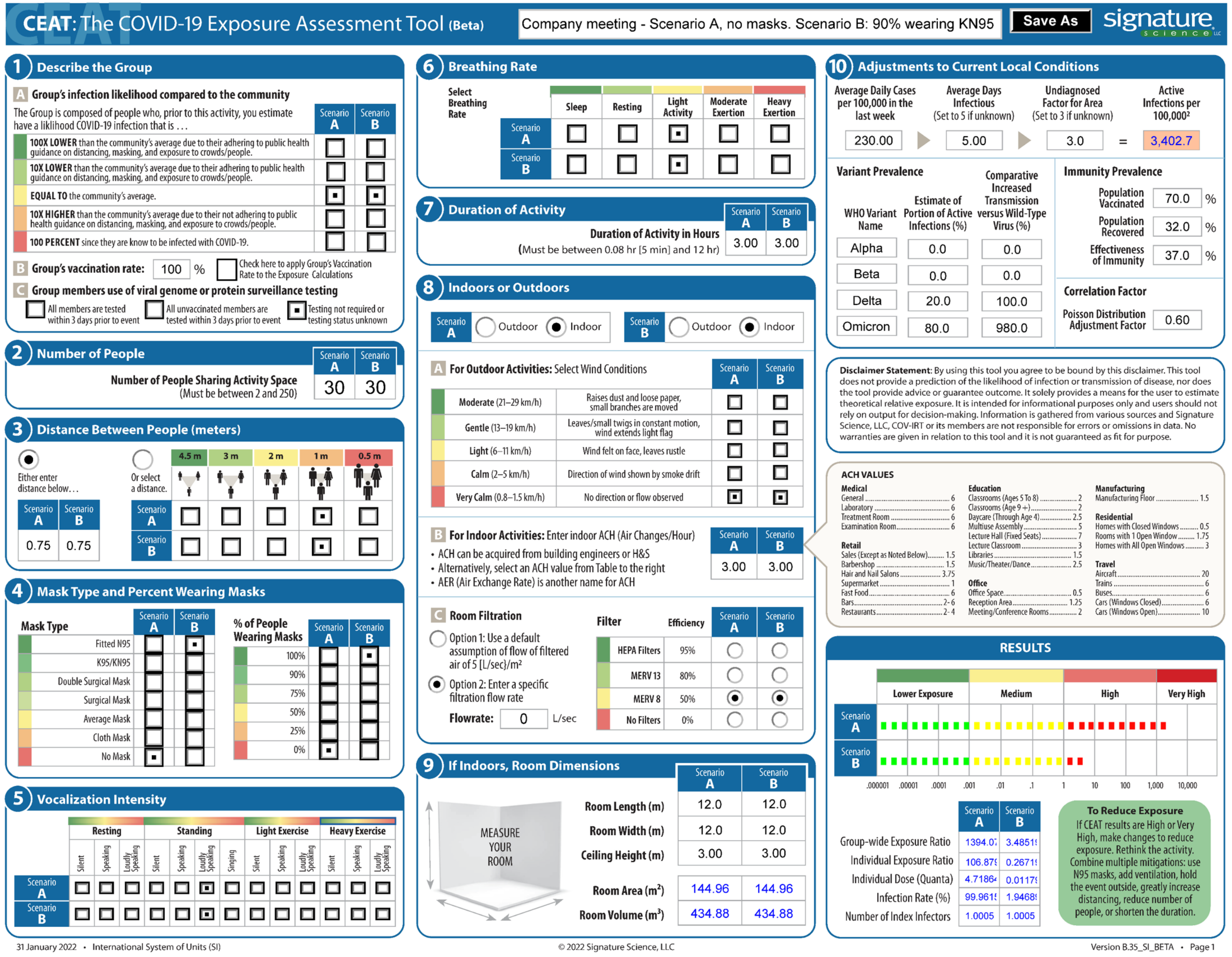


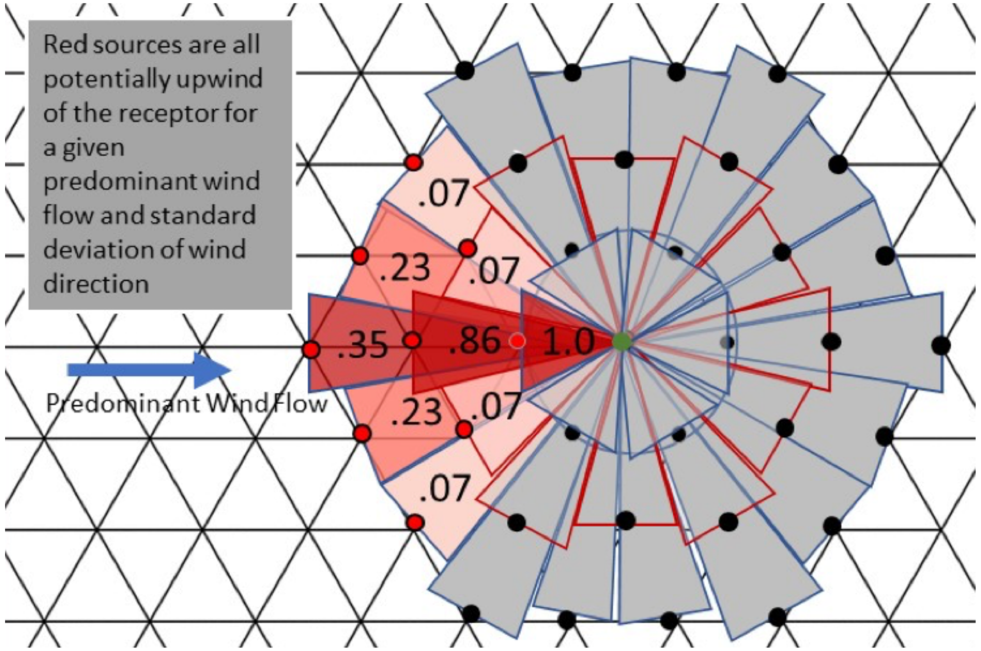
(a)
P4
P3
P2
P1
(b)
P1 P2 P3 P4
% Swept Out
0
10
20
30
40
50
60
70
80
90
100
0.5
1
2
4
8
16
32
Aerosol Diameter (microns)

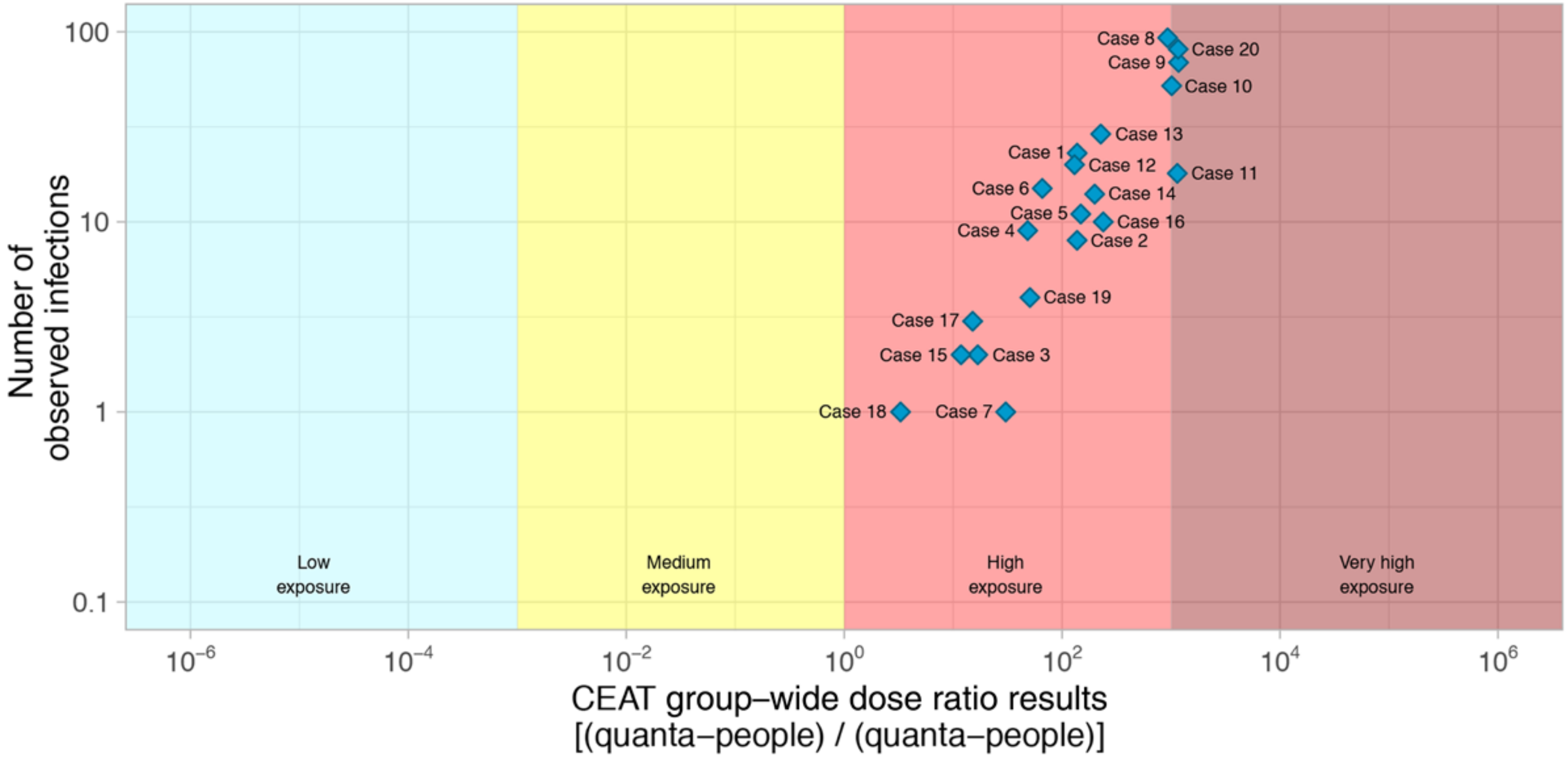


- Need substantial time to reach a statistical steady state, before aerosols can be injected
- 1.5 mins of real time takes 768 node hours on Frontera (~ 50,000 cpu hours)
- We need to run for at least 30 – 60 mins = 31,000 node hours
- Though it takes about 50,000 node hours to reach a statistically steady state, so each simulation of this size is costing about 100,000 node hours

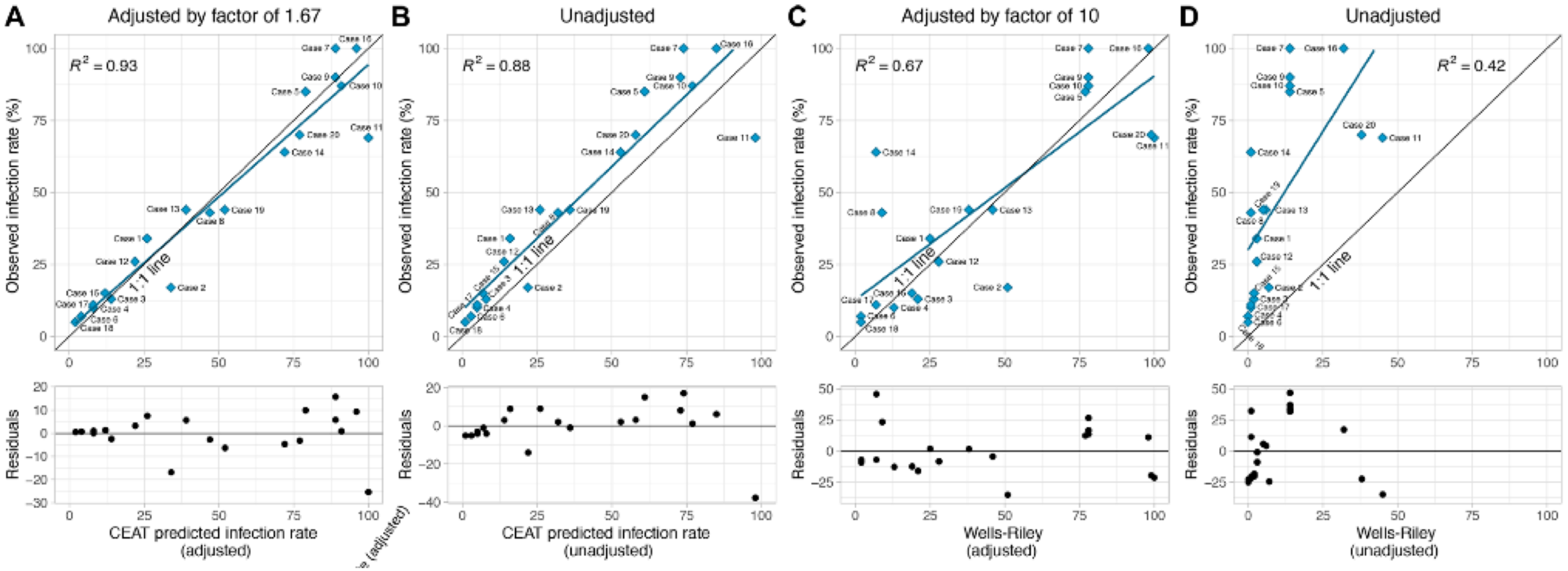
Fast & Accurate Prediction of Virus Loading in Heterogenous Indoor Environments： CEAT







CEAT's ability in predicting Super Spreader Events



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*)

Findpts implementation	GPU						CPU			
Migration	Yes			No			Yes		No	
particle count	100^3	150^3	200^3	100^3	150^3	200^3	100^3	150^3	100^3	150^3
Fluid Solve	98.2	98.1	98.5	99.2	98.2	107.5	97.9	98.7	101.2	100.1
Particle Creation	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Particle Update	3.6	8.5	19.1	18.6	60.8	146.1	277.0	910.2	288.3	953.9
- Copy fluid vel. to host	-	-	-	-	-	-	15.7	13.9	16.4	15.5
- findpts	2.7	6.4	14.3	8.9	29.0	69.1	225.3	746.5	234.1	775.9
- - Memcpy	0.4	0.7	1.2	0.8	1.8	4.2	-	-	-	-
- - Kernel	1.8	4.9	11.3	1.9	6.4	14.6	219.7	735.7	220.4	734.7
- migration	0.1	0.1	0.3	-	-	-	0.1	0.2	-	-
- findpts_eval	0.6	1.3	3.1	9.4	31.0	74.9	49.7	158.5	54.0	177.1
- - Memcpy	0.2	0.4	0.9	0.3	1.0	2.0	-	-	-	-
- - Kernel	0.5	0.9	2.2	0.3	0.8	1.4	49.6	158.5	43.2	141.9
- Advance position	0.2	0.5	1.2	0.2	0.5	1.3	0.2	0.5	0.1	0.5
- Barrier	0.0	0.1	0.2	0.1	0.3	0.8	1.8	4.4	0.1	0.3

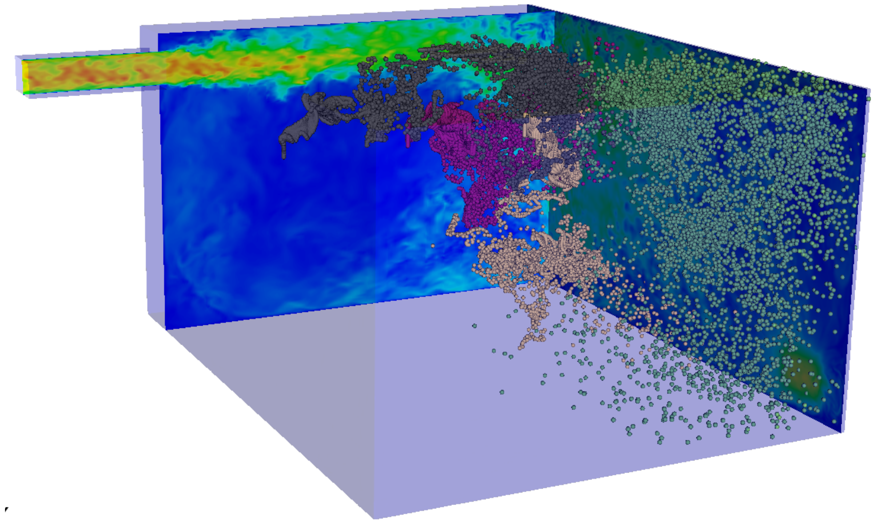
Conclusions and Future Directions from Room-scale Simulations

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

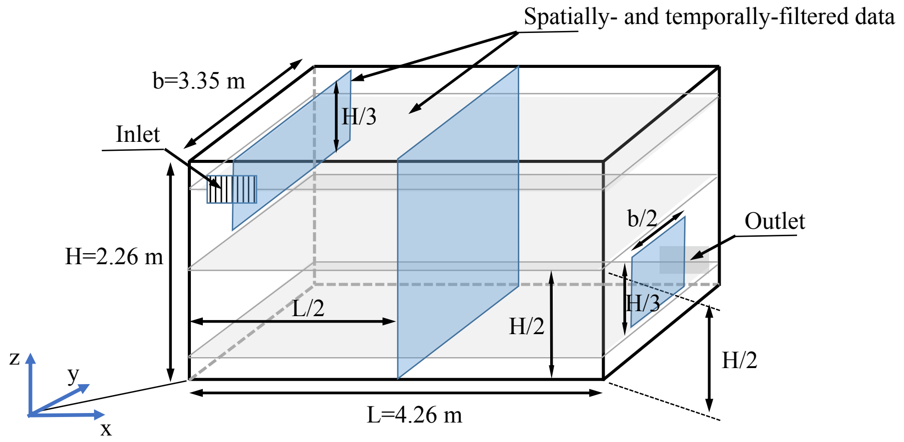
- **These simulations will be used as benchmark results to compare/improve lower-fidelity models (e.g. RANS based)**

- **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**

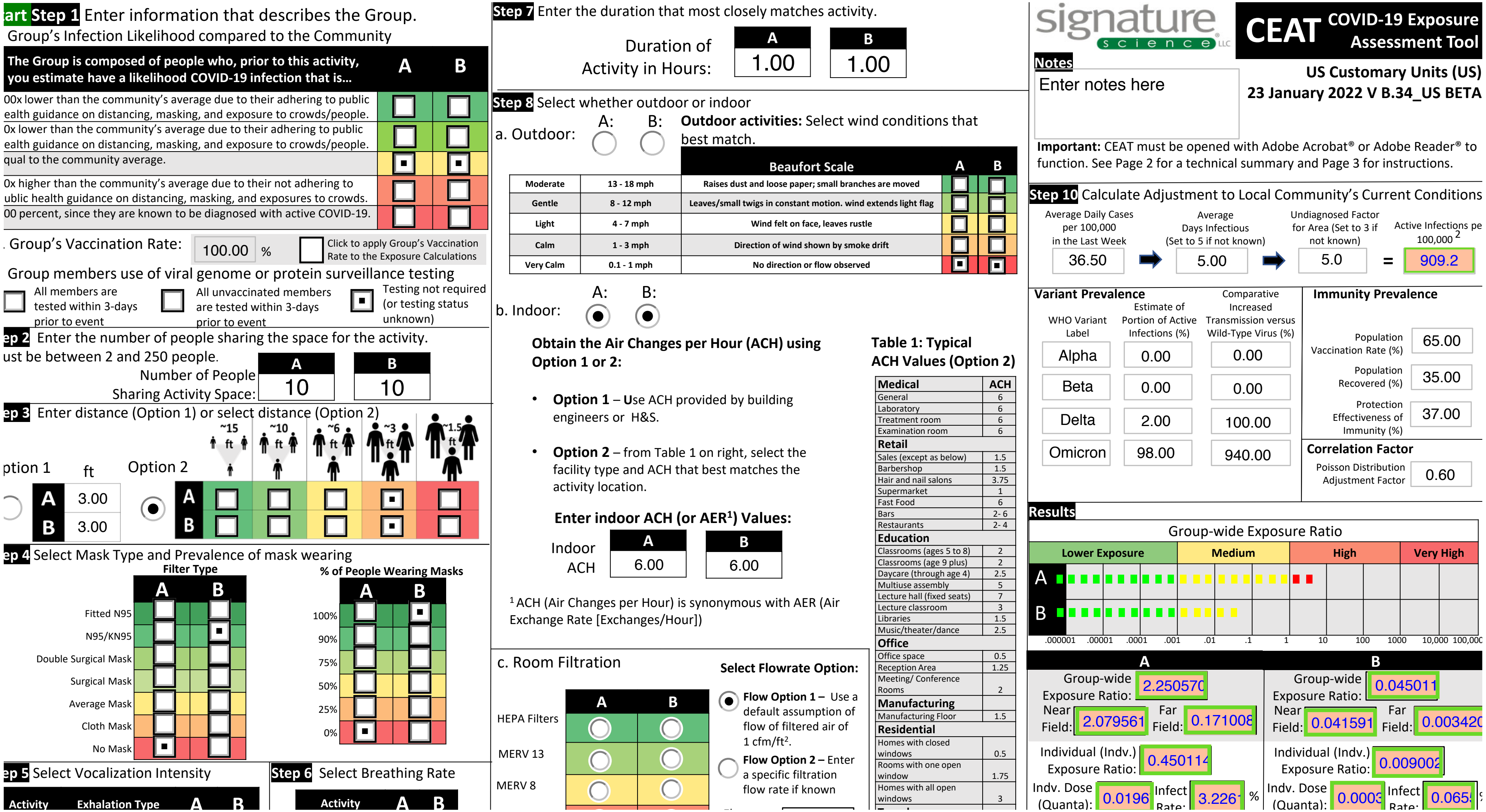


Basic Measurement Setup

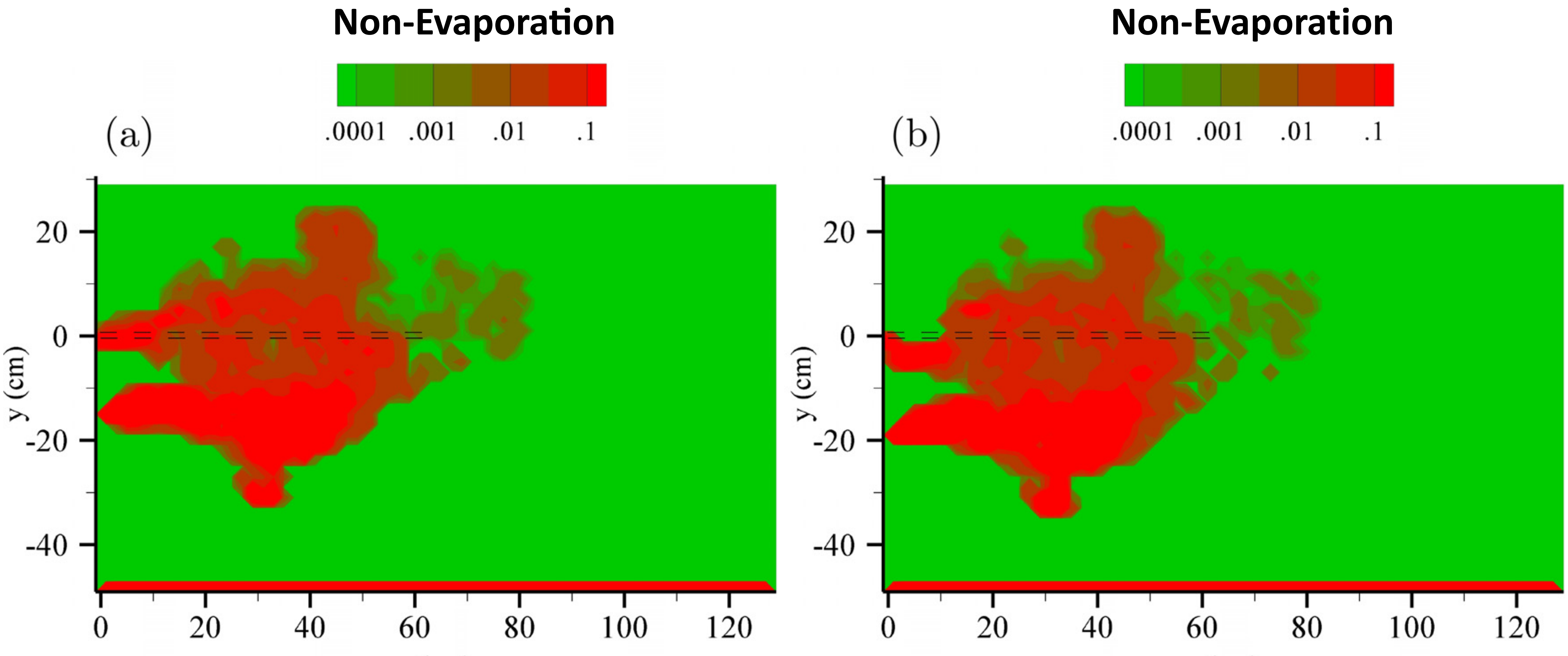


Temporal states: Development and Stationary

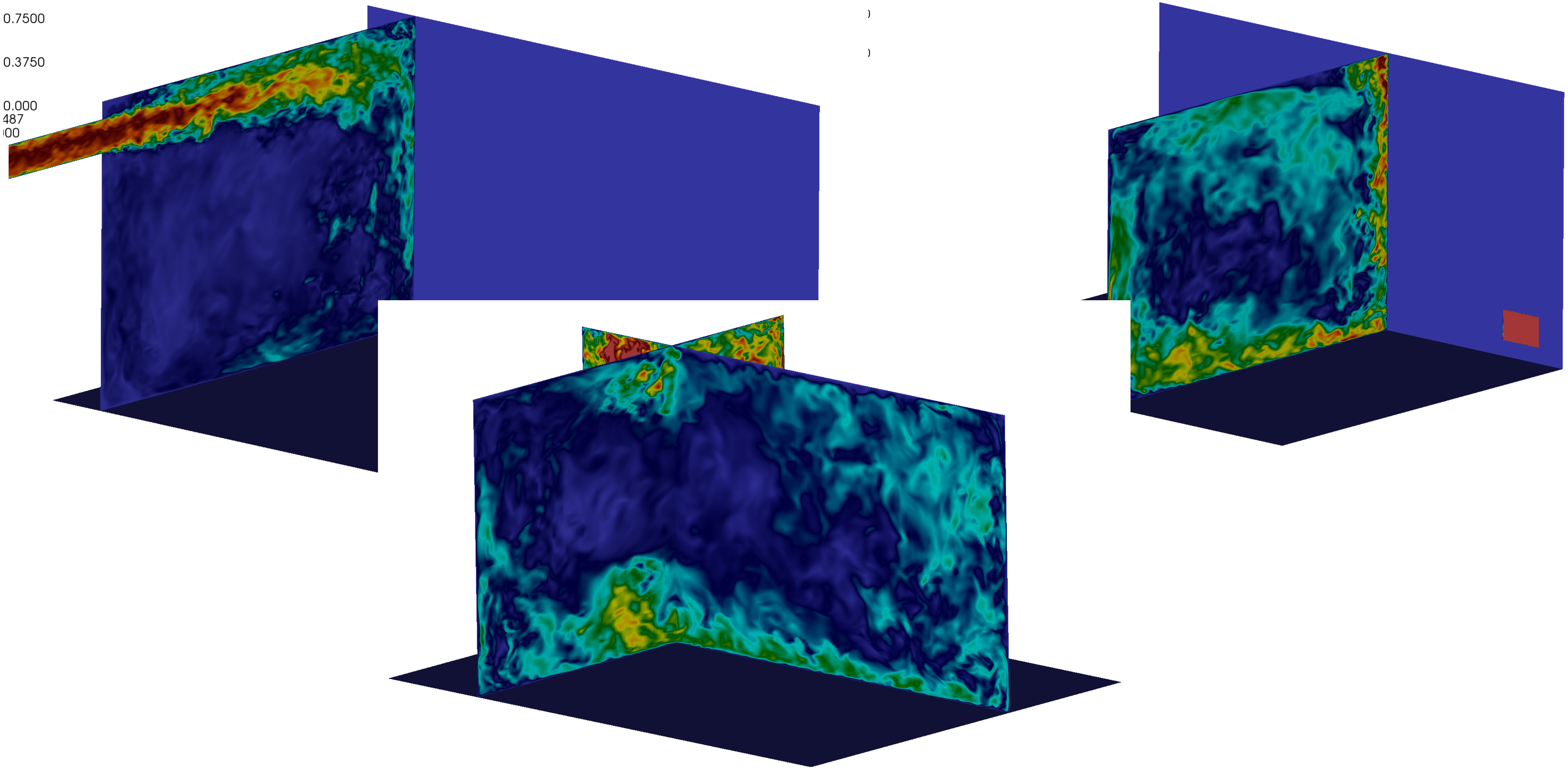
Final Objective: Development of a robust Covid-19 Exposure Assessment Tool (CEAT)

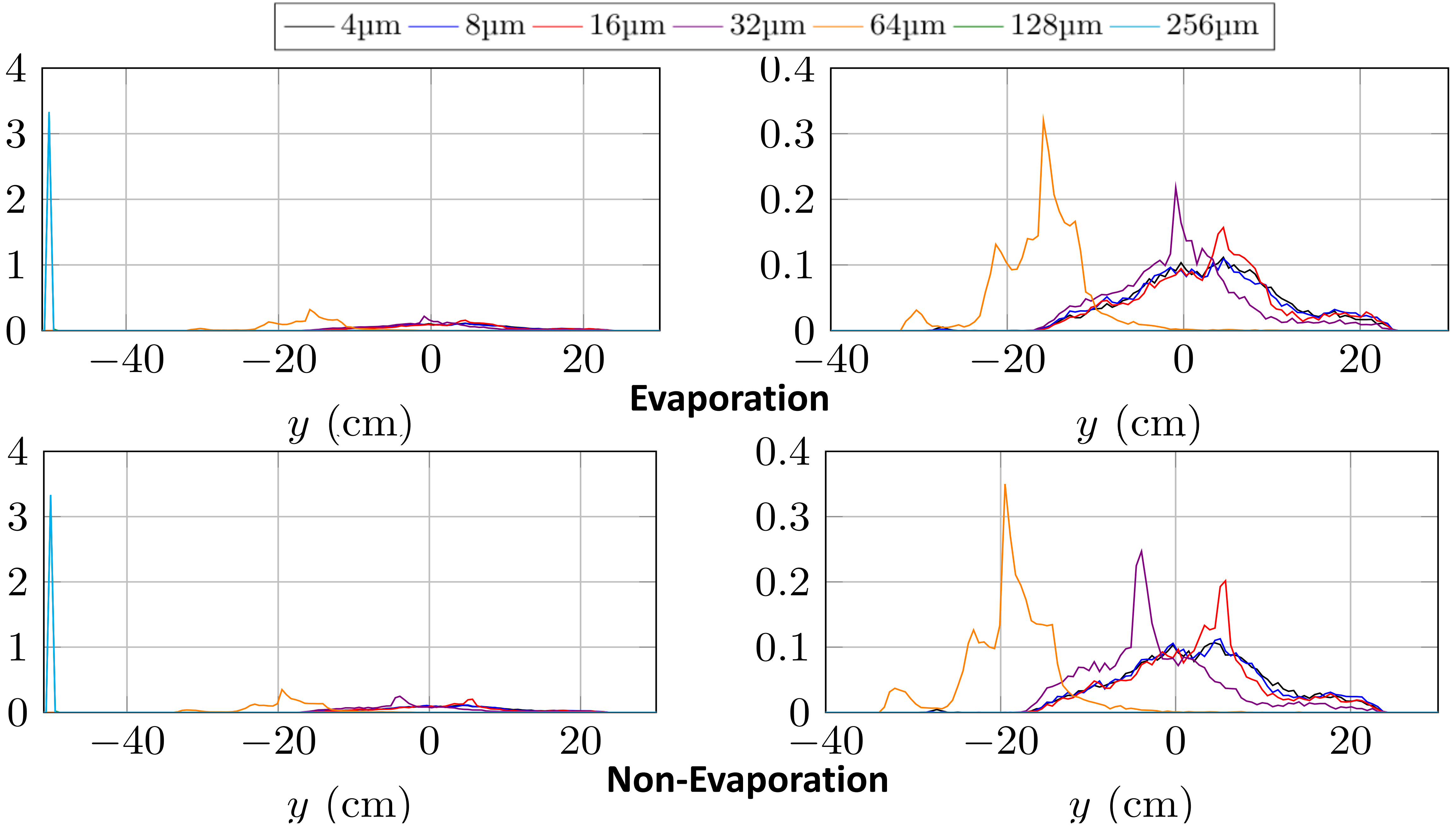


Potential Viral Load (based on particle size and concentration) from the Cough



Room scale flow structure at 6 ACH





4µm 8µm 16µm 32µm 64µm 128µm 256µm
Evaporation
Non-Evaporation
y (cm)
y (cm)
y (cm)
y (cm)