

High-Performance Computational Fluid Dynamics for Virus Propagation in Closed Ventilated Domains



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PRACE

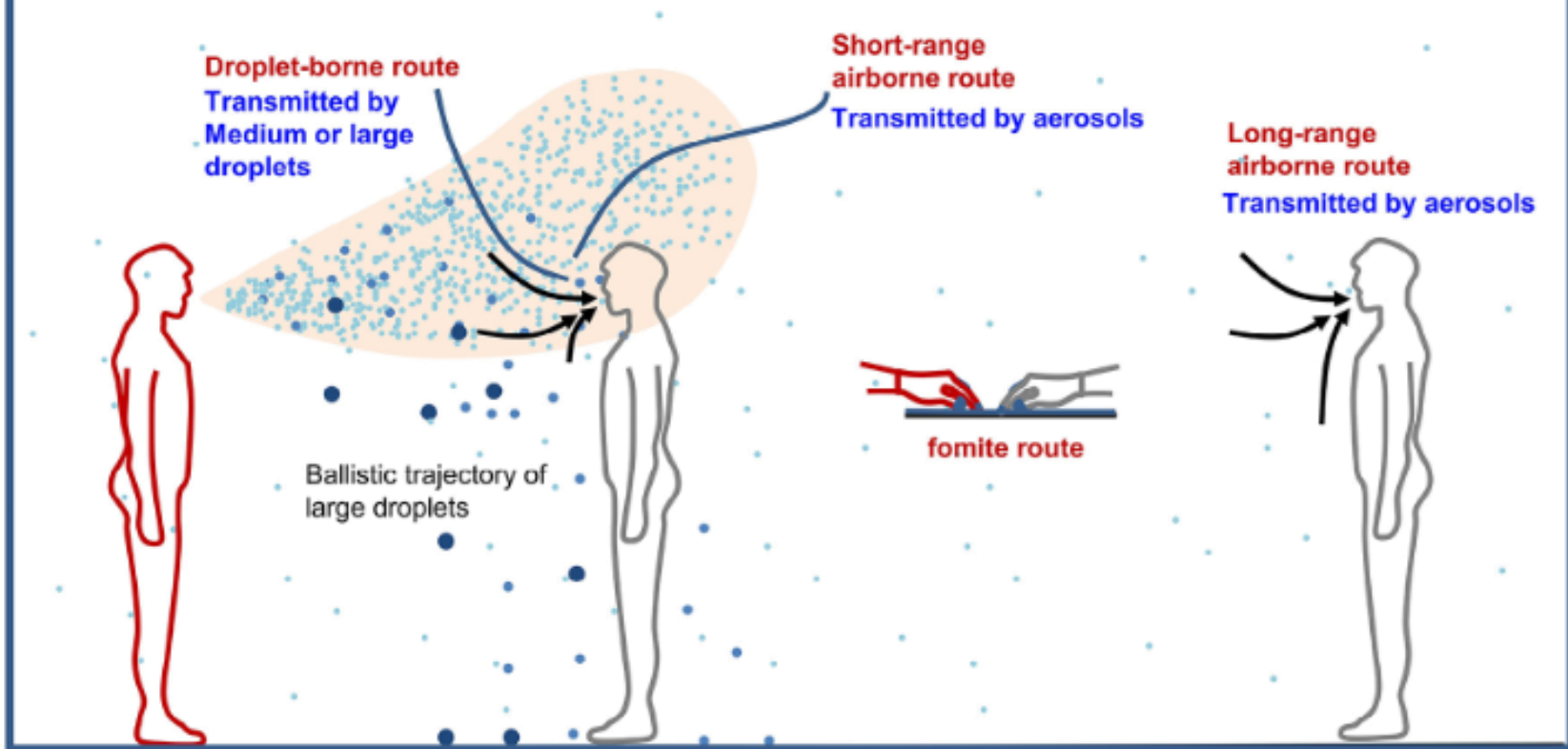
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 **GENCI**

Le calcul intensif au service de la connaissance

Context – Airborne virus propagation

J. Wei, Y. Li, American Journal of Infection Control 2016, 44, S102.



- Large droplets ($>100 \mu\text{m}$) : Fast deposition due to the domination of gravitational force
- Medium droplets between 5 and $100 \mu\text{m}$
- Small droplets or droplet nuclei, or aerosols ($< 5 \mu\text{m}$): Responsible for airborne transmission

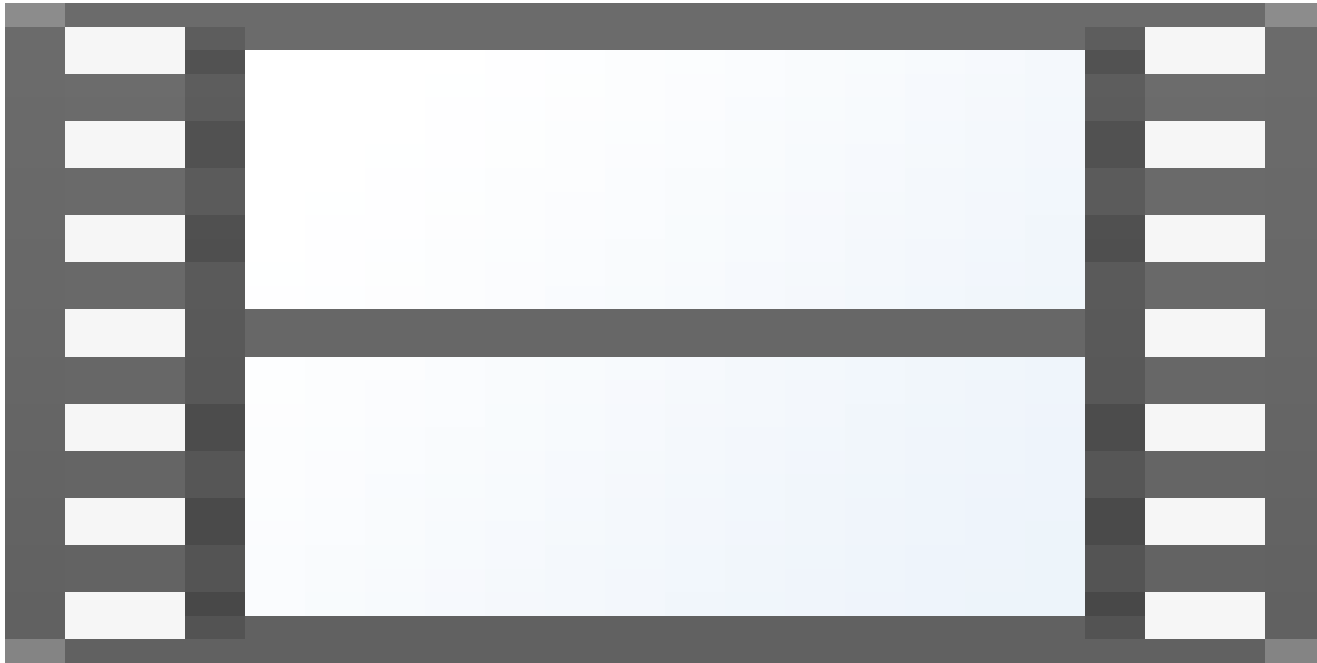
➔ Where the respiratory droplets migrate : **Computational Fluid Dynamics**

➔ How many time the virus is active : **Biology**



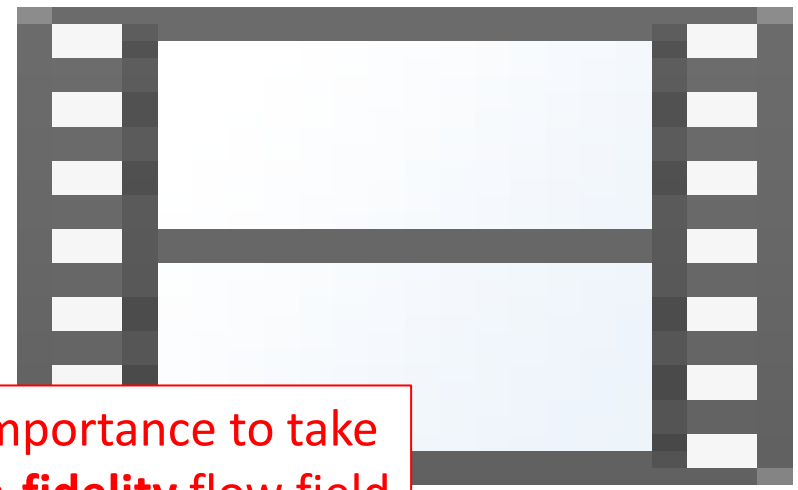
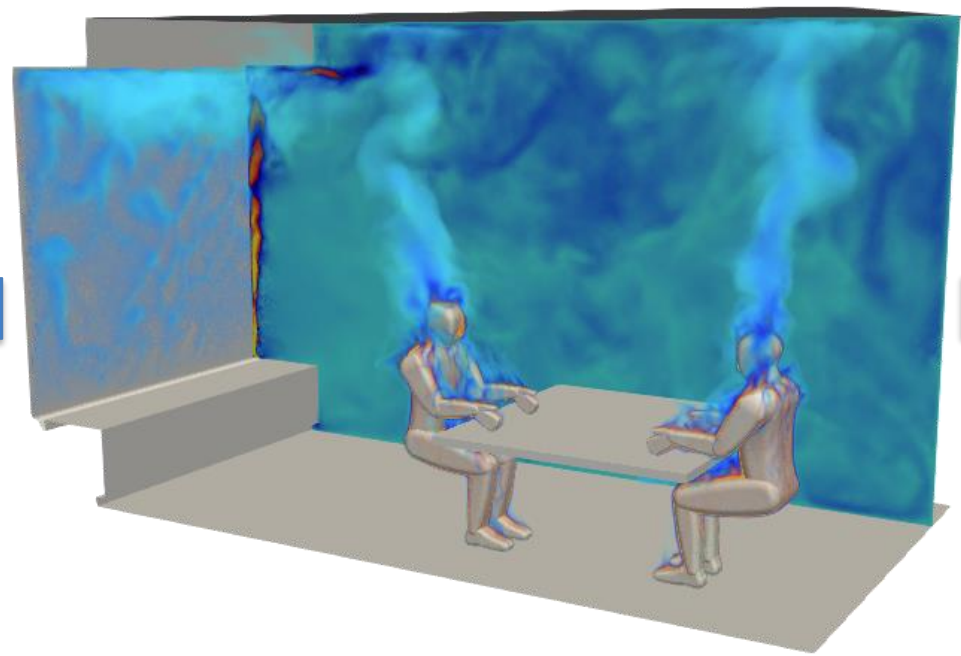
Context – Airborne virus propagation

We started to play with short-range airborne route → ~ seconds



What happen in enclosed ventilated spaces when considering long-range airborne routes → ~ Hours

Requirement for high-fidelity flow predictions



It is of primary importance to take into account **high-fidelity** flow field (ventilation, buoyancy ...)

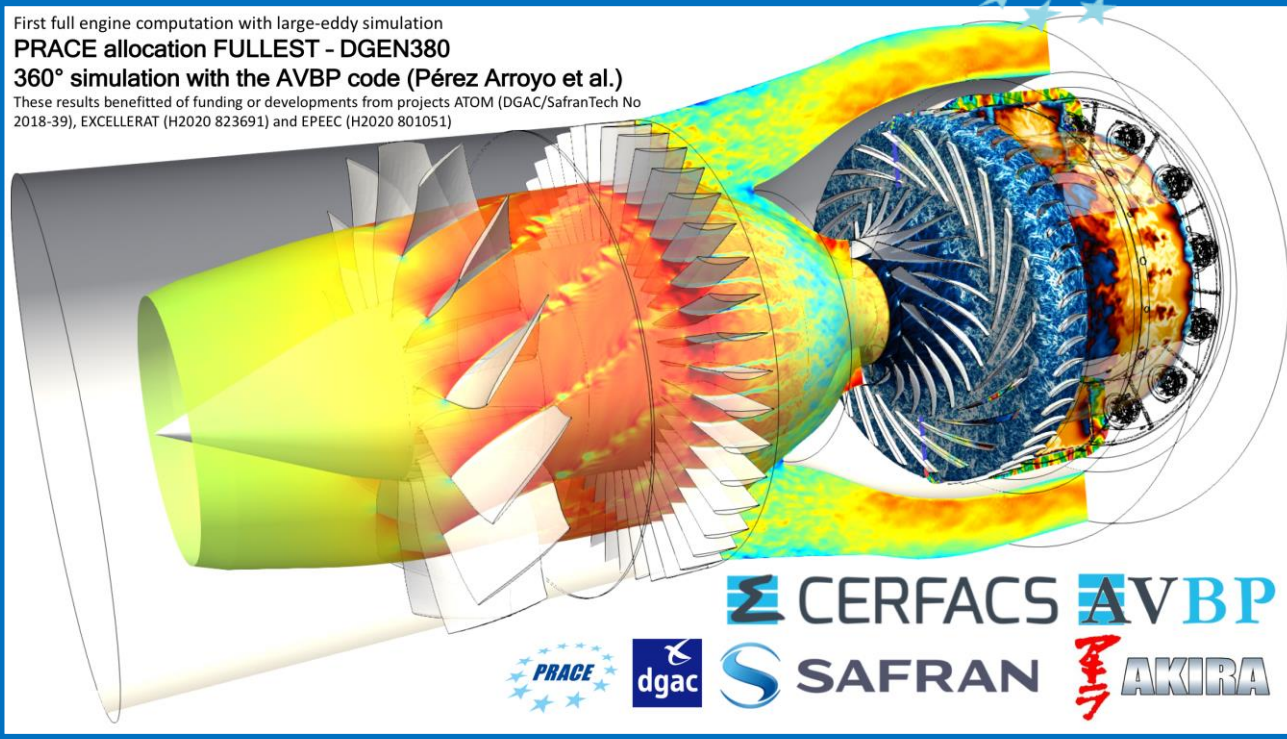
Computational solution

AVBP Solver - CERFACS



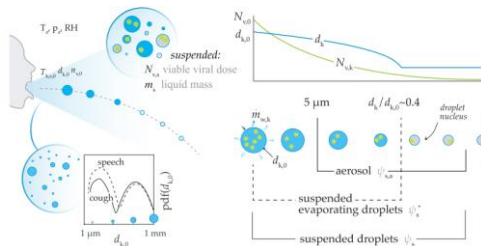
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First full engine computation with large-eddy simulation
PRACE allocation FULLEST - DGEN380
360° simulation with the AVBP code (Pérez Arroyo et al.)
These results benefitted of funding or developments from projects ATOM (DGAC/SafranTech No 2018-39), EXCELLERAT (H2020 823691) and EPEEC (H2020 801051)



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Droplets and virus models

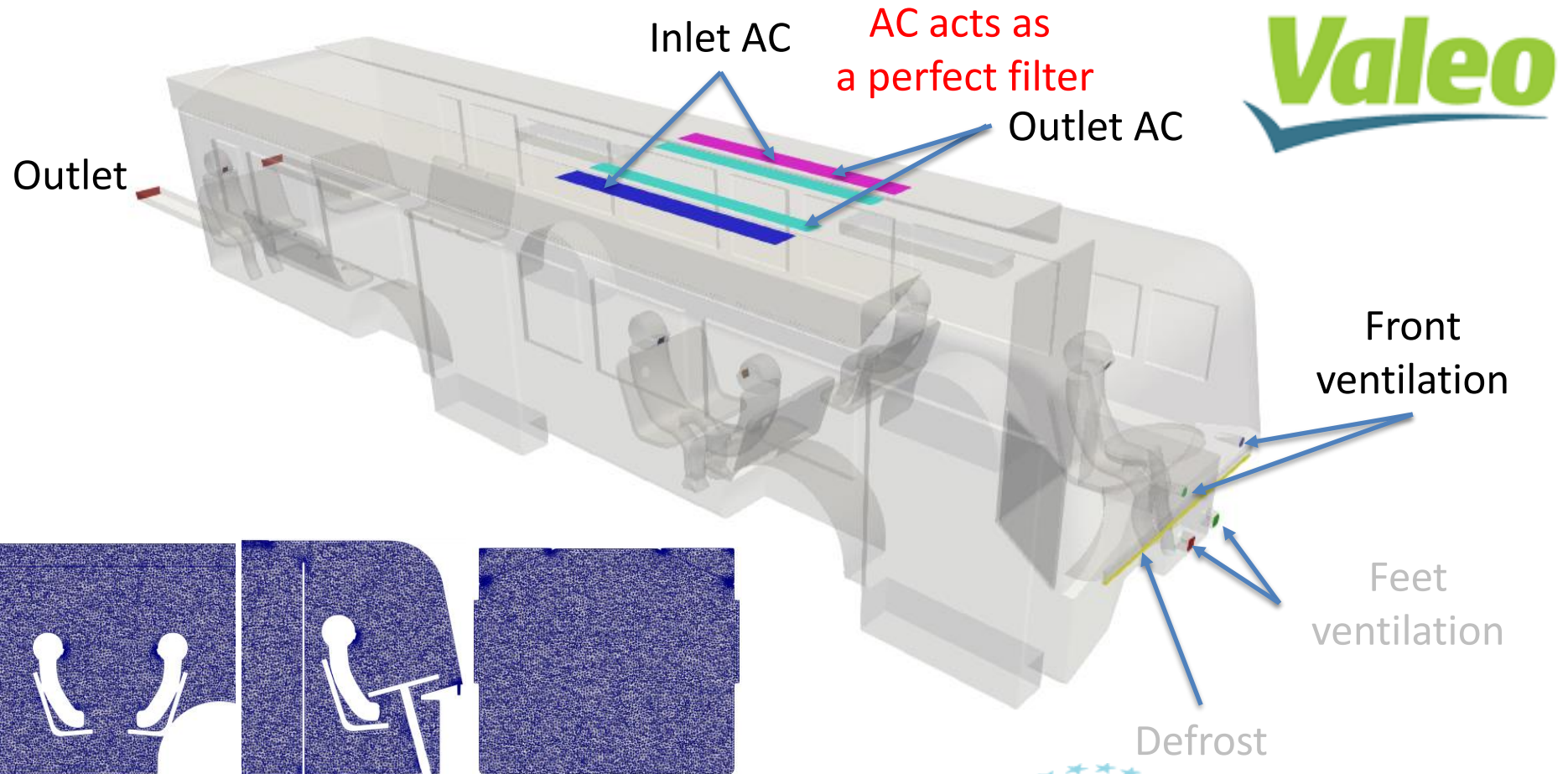


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Respiratory droplets dispersion during long times

- High-fidelity Large Eddy Simulations
- Droplet dispersion on mean fields

Applications – Bus – Setup



- 40 M cells
- TTGC numerical scheme [Colin and Rudgyard 2000]
- WALE sub-grid scale model [Nicoud and Ducros 1999]

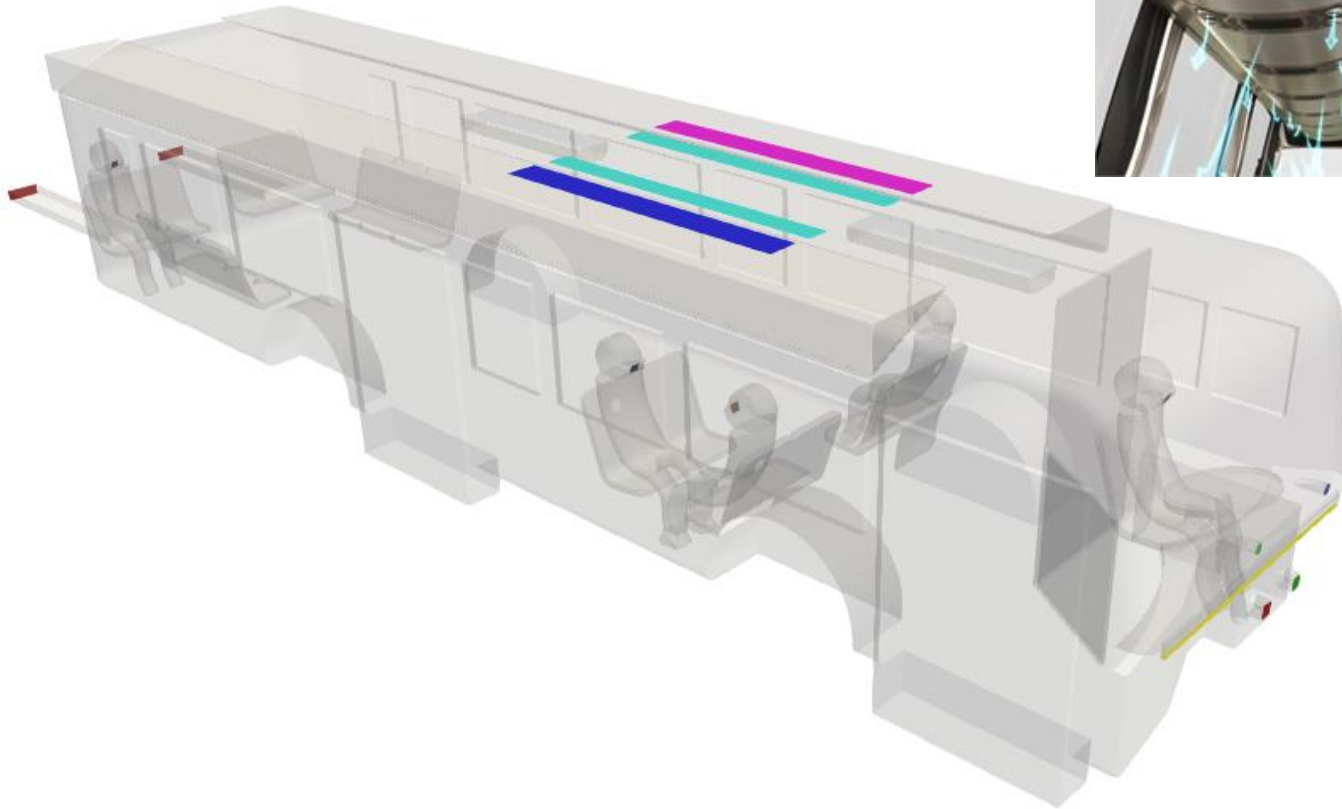


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Applications – Bus – Setup



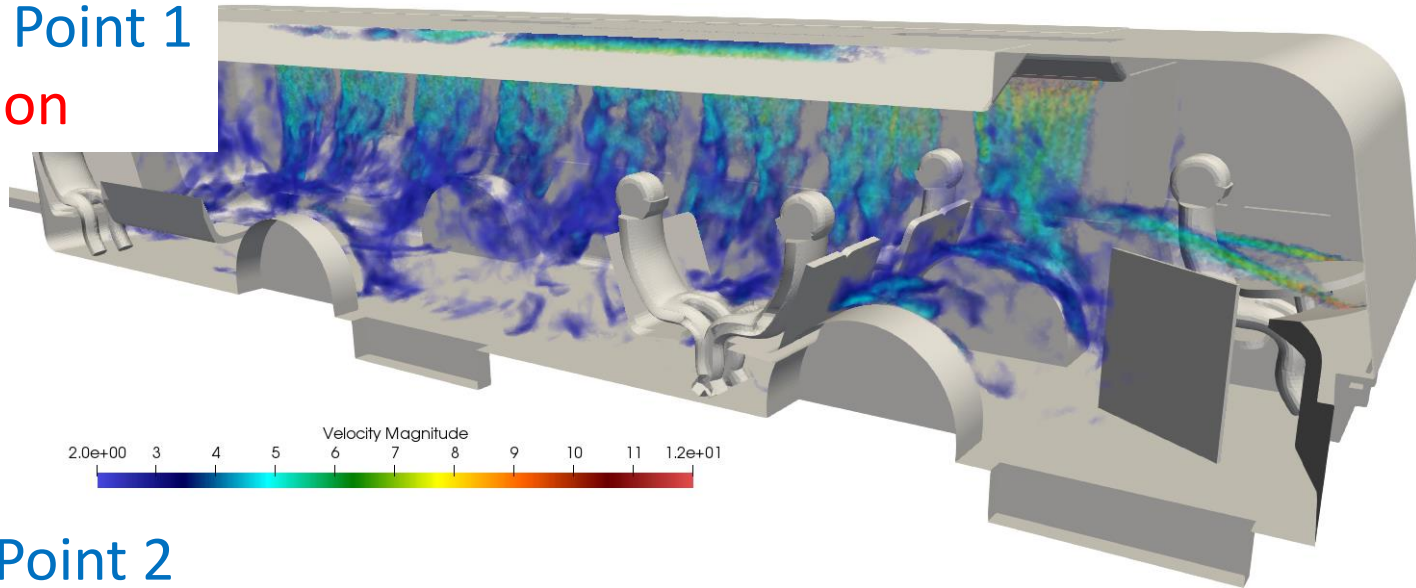
AC acts as a perfect filter:
Idealization of a air
purification system



https://www.valeo-thermalbus.com/eu_en/Innovation/UV-air-purification

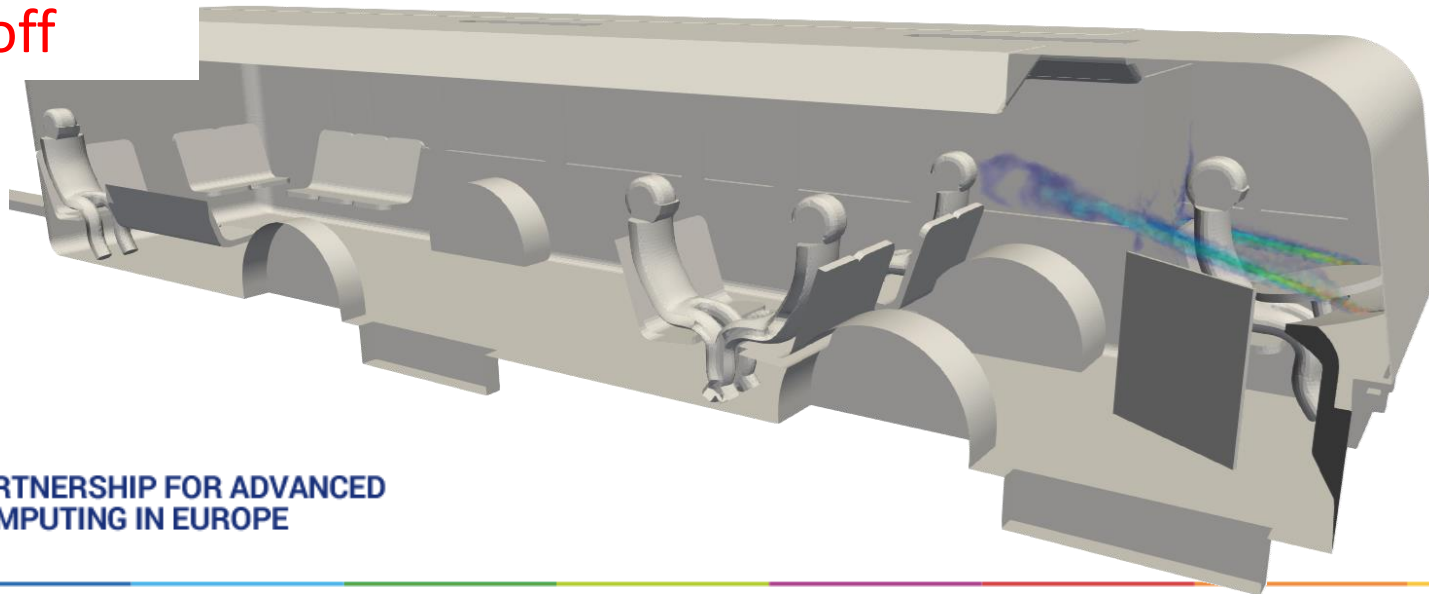
Operating Point 1

→ AC on



Operating Point 2

→ AC off



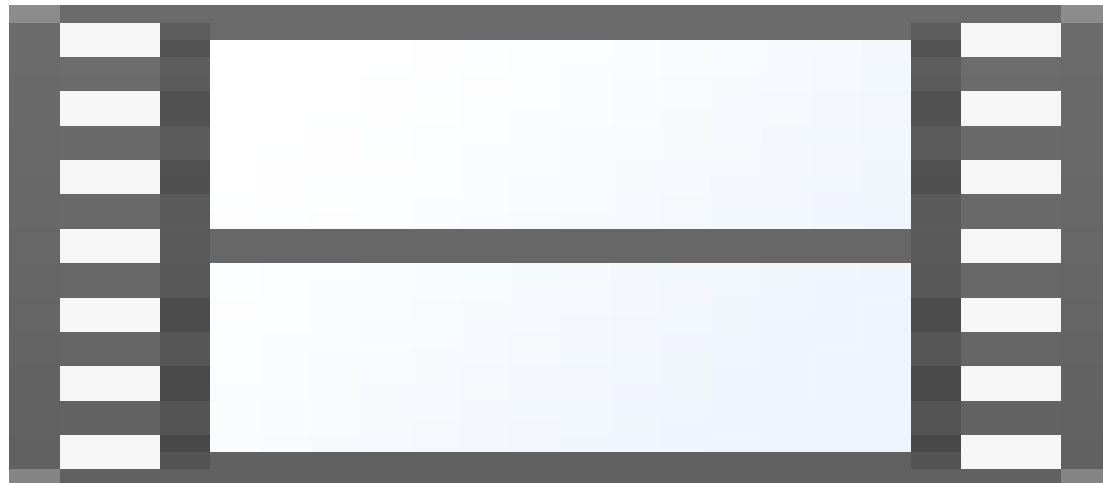
Operating Point 1

→ AC on



Operating Point 2

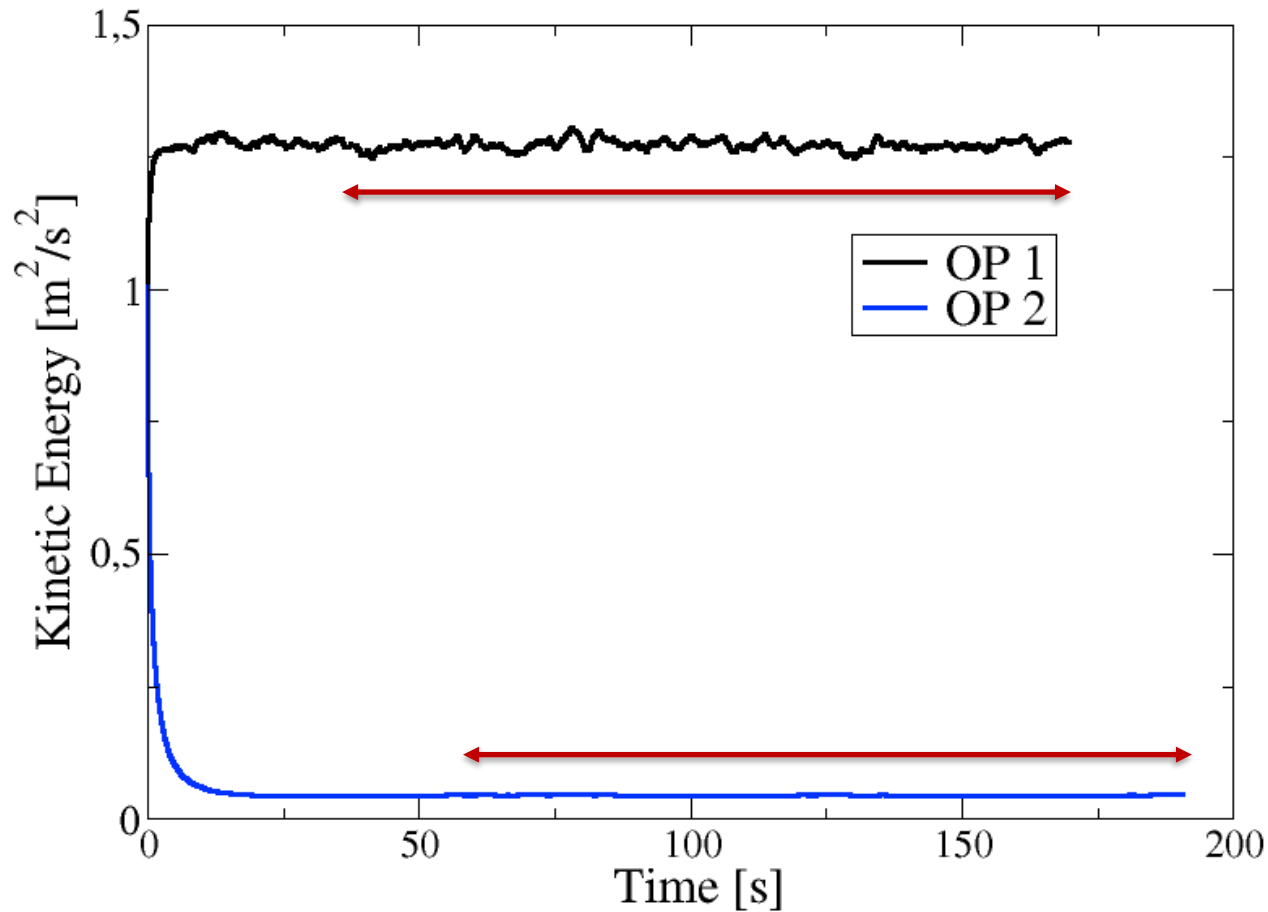
→ AC off



Very different
flow fields and
turbulent activity

Convergence of the gaseous fields:

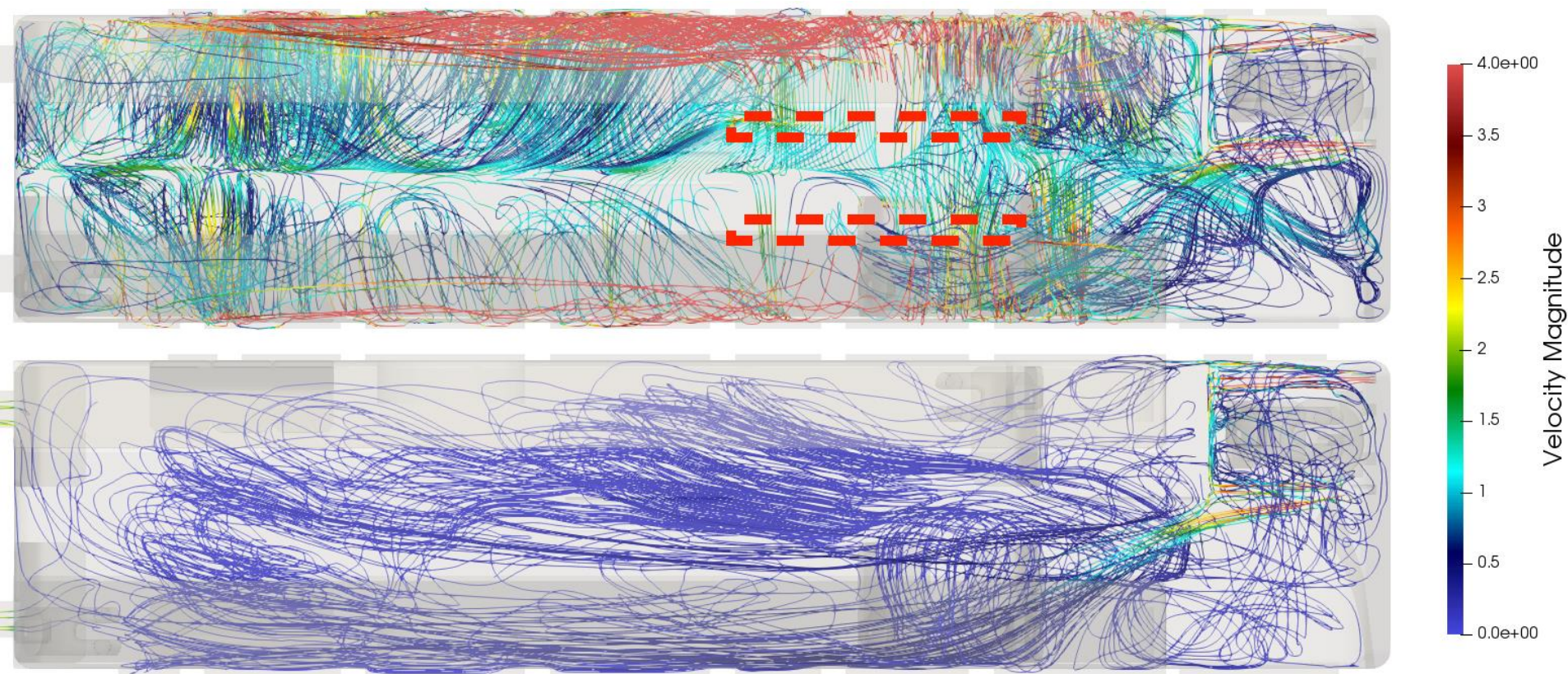
- ➔ Transient evacuation in 15 s for OP1 and 40 s for OP2
- ➔ Time averaged on the last 130 seconds



Very different flow organization

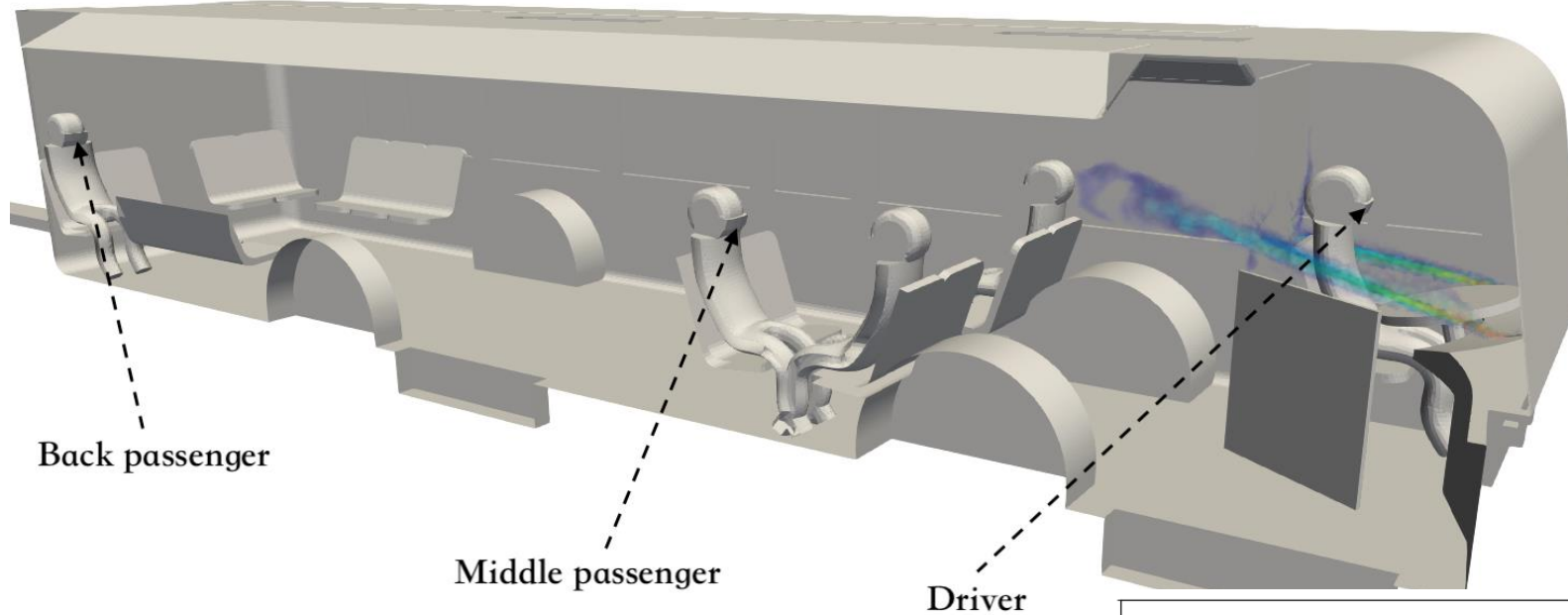
➔ impact on respiratory droplet dispersion

Operating Point 1



Operating Point 2

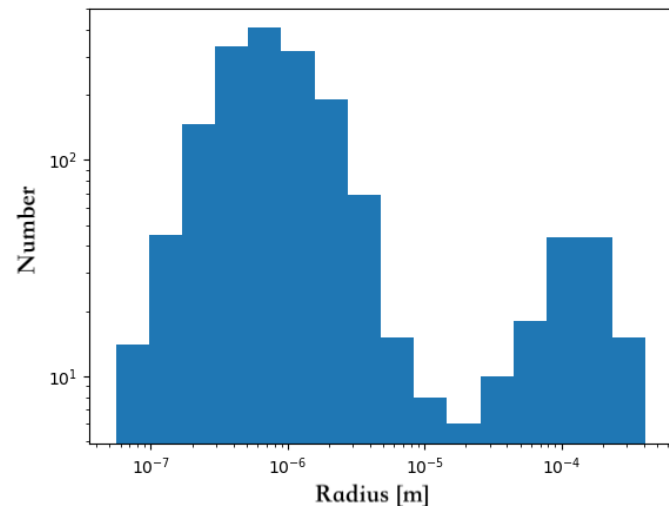
Three respiratory droplet dispersion simulations per OP



Two mean LES fields

→ 6 droplet dispersion computations

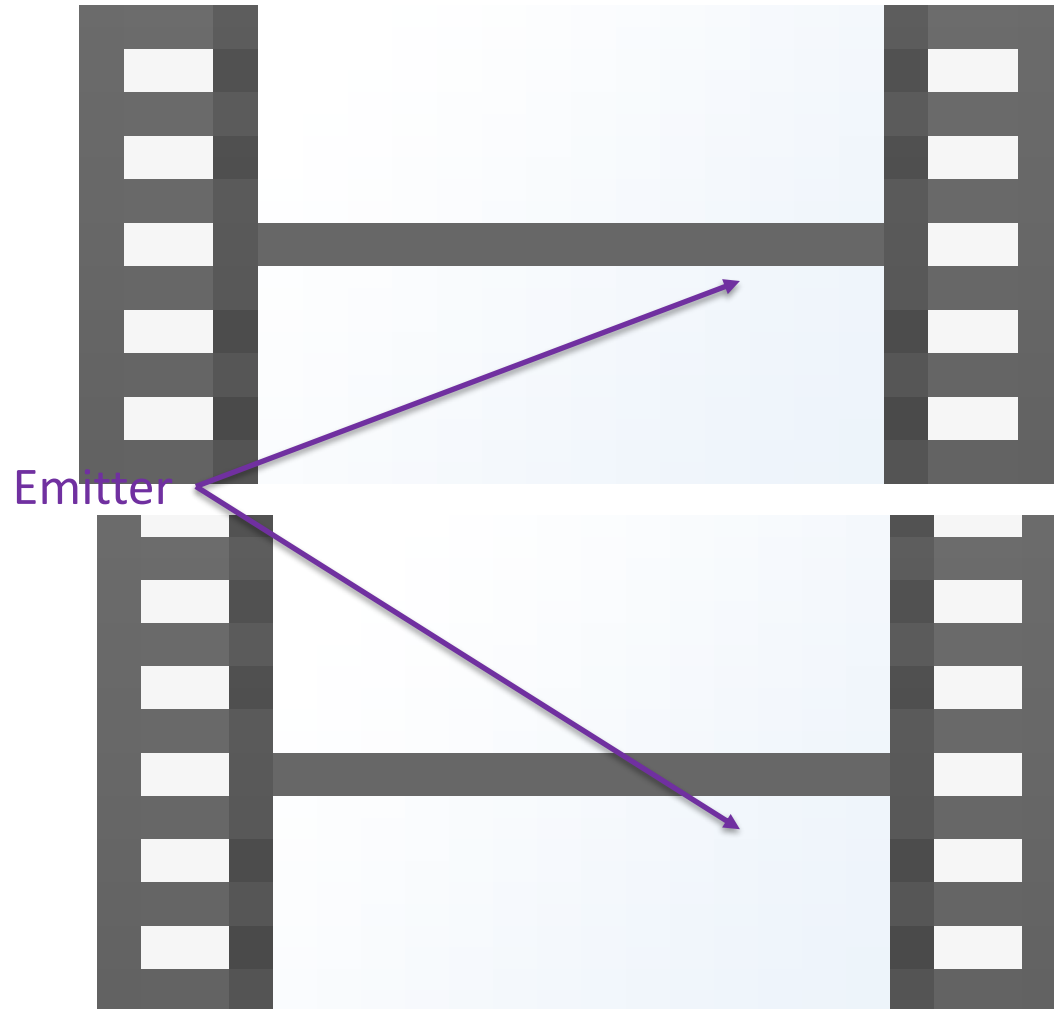
Respiratory droplet distribution
(de Oliveira et al. 2020)



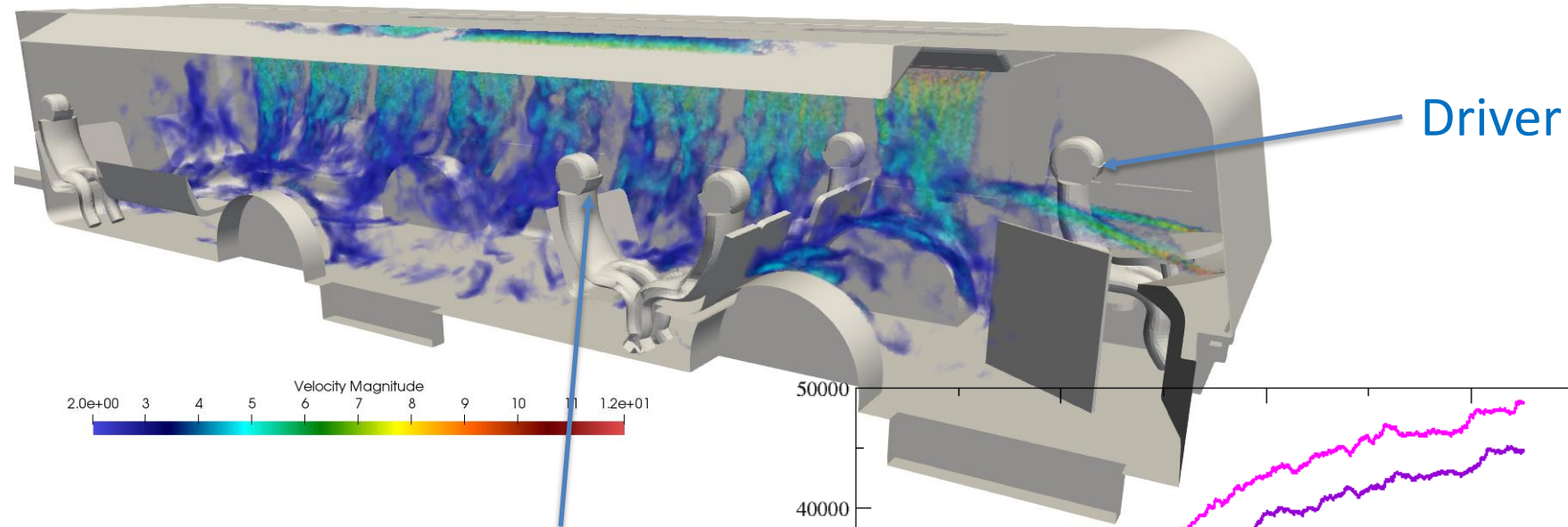
After One hour respiratory droplet dispersion simulation

Operating Point 1

Droplets colored by diameter
Small Big



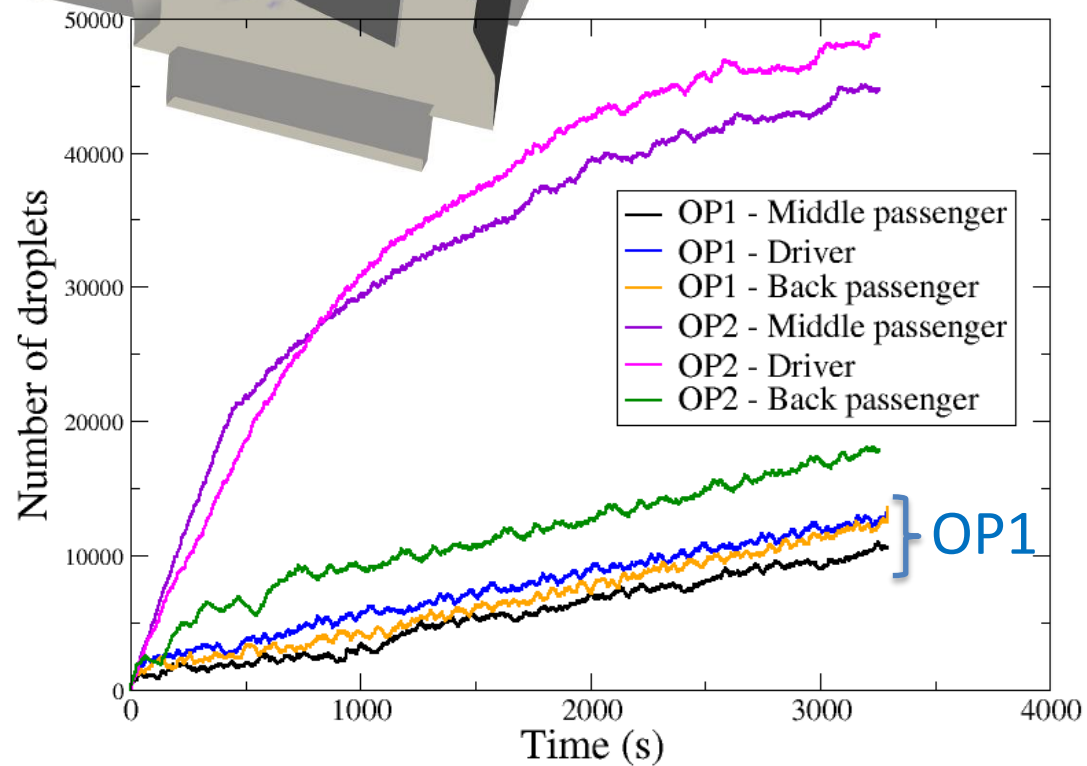
Operating Point 2

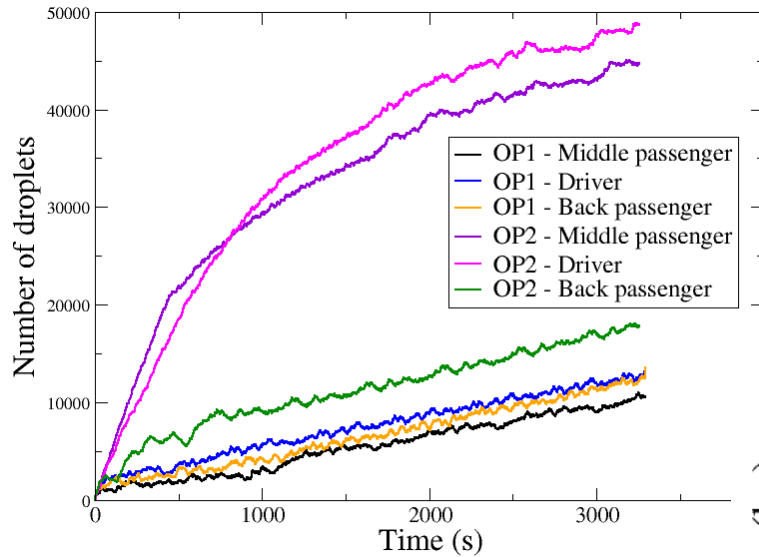


Back Passenger

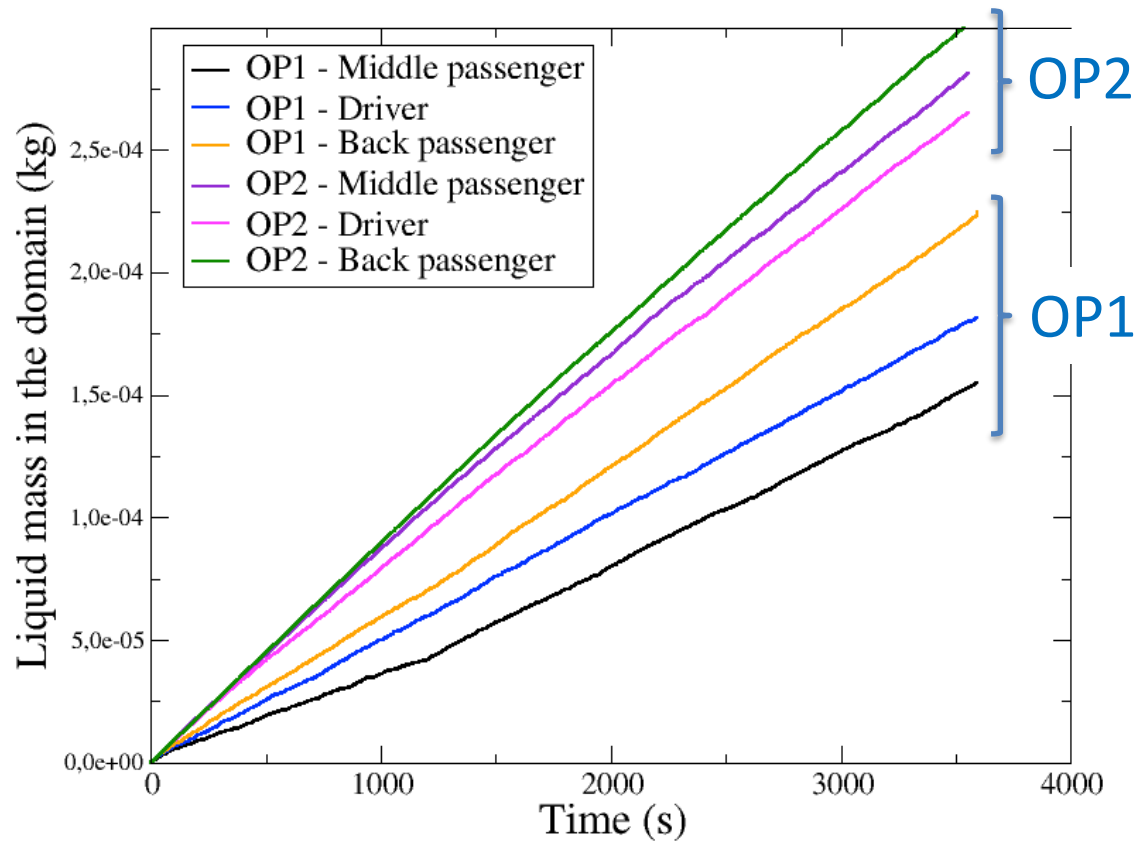
Middle passenger

➔ No equilibrium after one hour
 ➔ Important droplet accumulation in OP2





Small droplet (aerosols) are preferentially evacuated

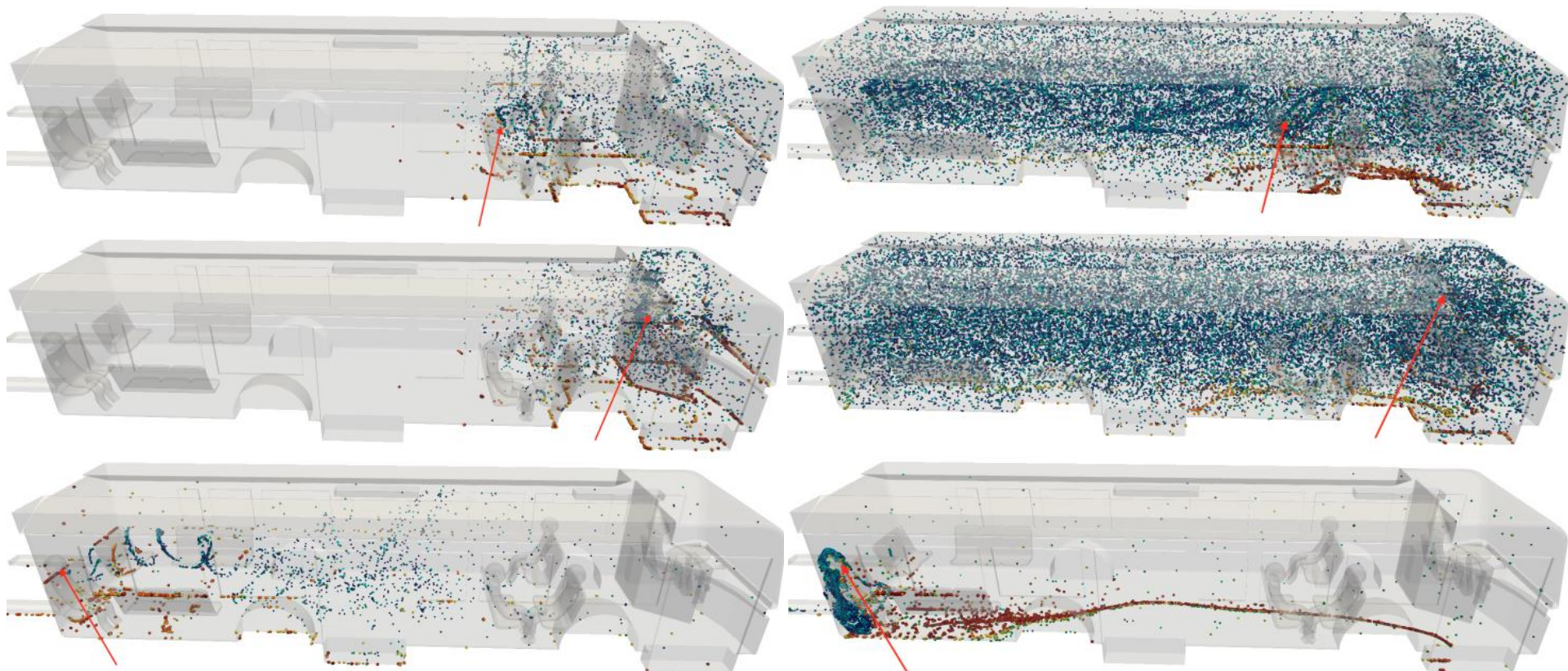


Operating Point 1

→ AC on

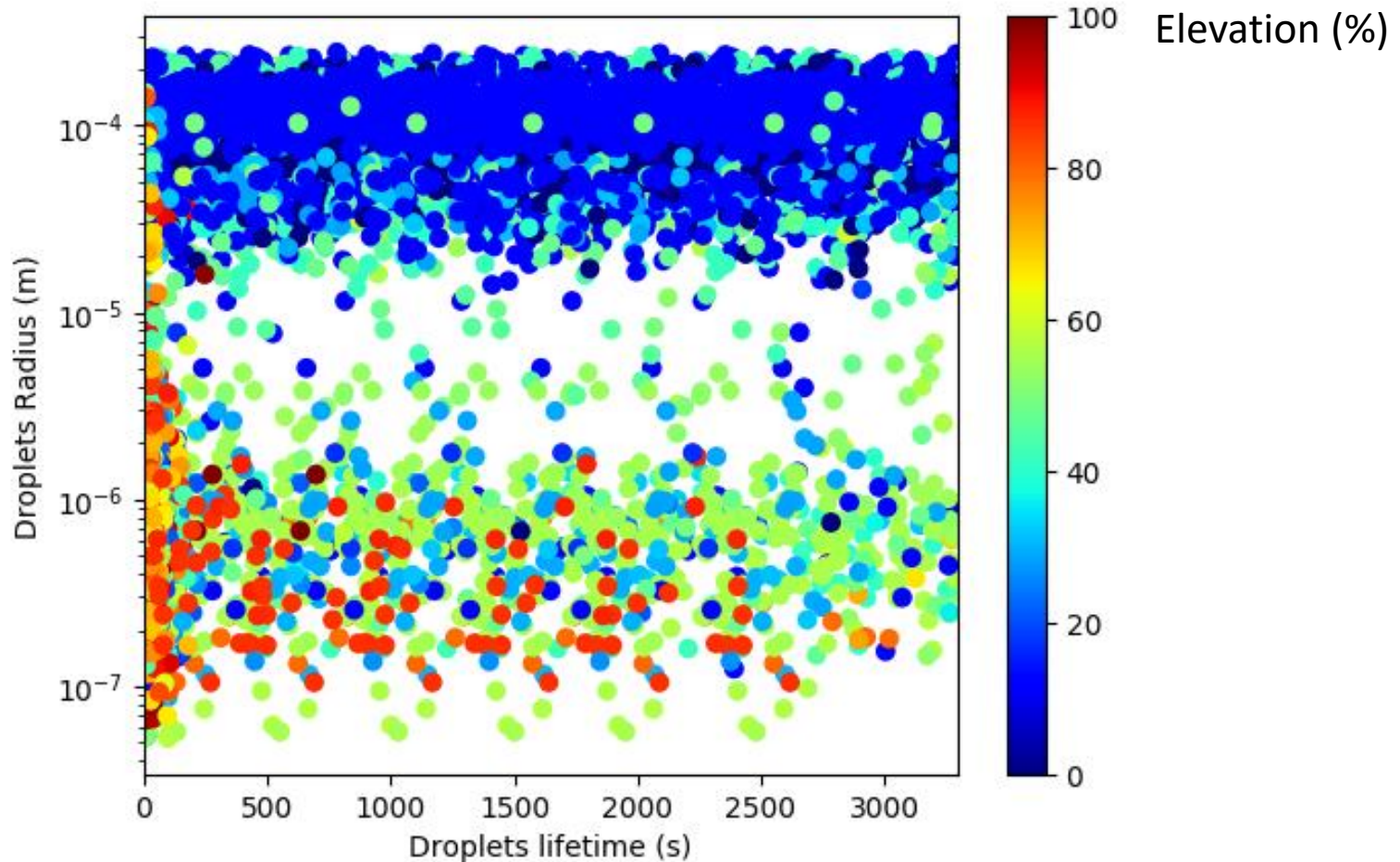
Operating Point 2

→ AC off

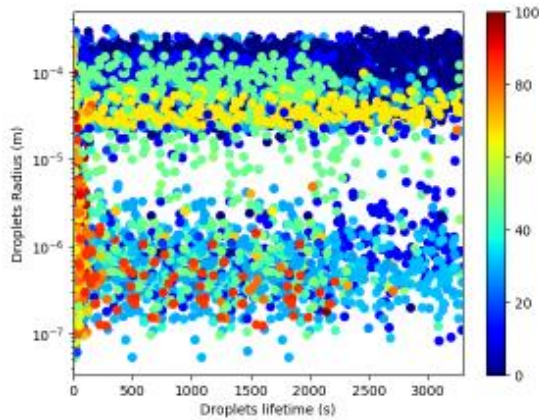


AC allows to evacuate small droplets and avoid dispersion in all the bus

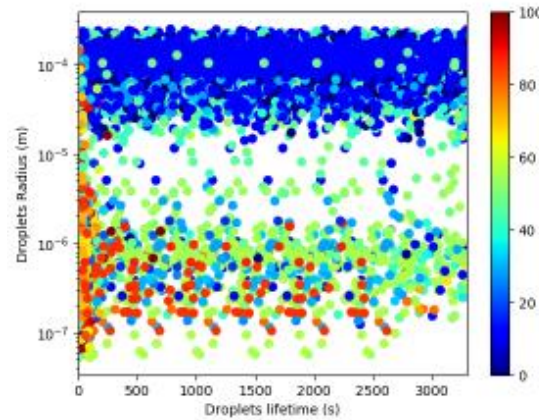
Scatter plot of droplet lifetime VS radius colored by elevation in the bus (%) at the end of the simulations



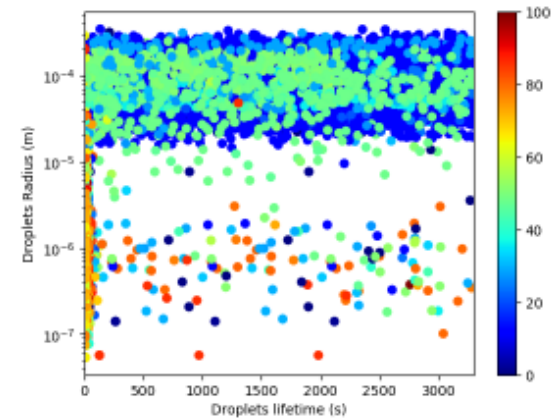
OP1 - Middle Passenger



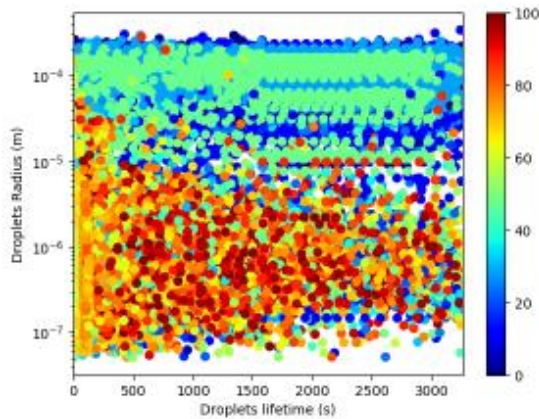
OP1 - Driver



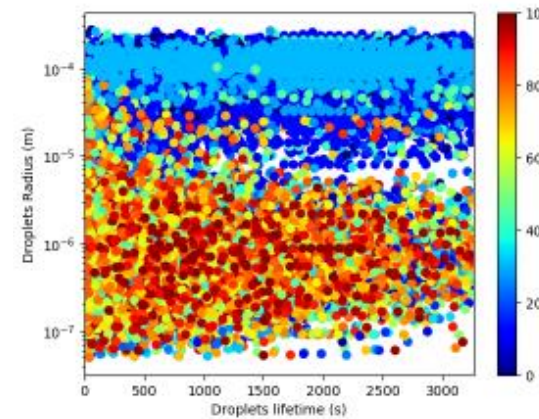
OP1 - Back Passenger



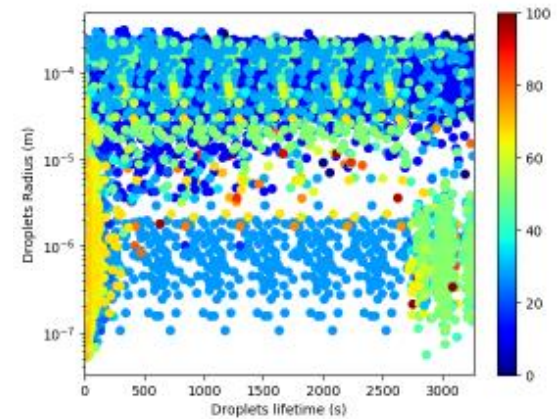
OP2 - Middle Passenger



OP2 - Driver



OP2 - Back Passenger



Droplet lifetime (s)

AC allows to evacuate small droplets and avoid dispersion in all the bus

Take home messages

- **High-fidelity** Computational Fluid Dynamics is able to discriminate **flow behavior** in different scenarios and thus **turbulent droplet dispersion** and help to design systems to provide **safer environments**

Case	Mesh Size	Physical time (s)	CPU hours	Droplet time (s)	CPU hours	Acceleration
Bus	40 M	130	500 000	3600	2 000	7 500



Need to continue to work on

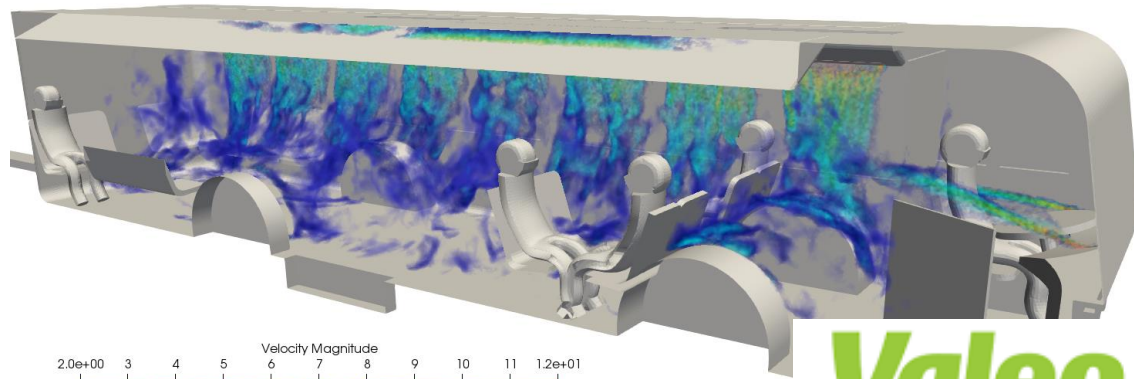
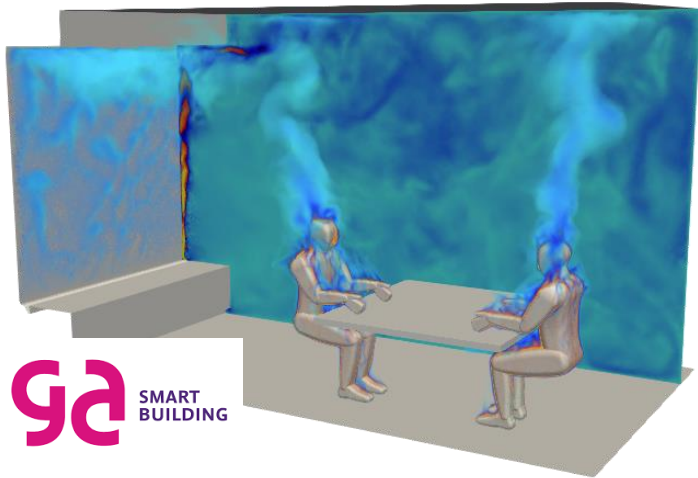
- Turbulent droplet dispersion model
- Biology aspects: virus loading and lifetime
- mitigation solutions modeling

How important has HPC been for COVID research?

- CPU hours provided by PRACE and GENCI helped us to rapidly compute flow fields in many configuration and adjust some numerical models



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