Adaptive machine-learning tool for computationally efficient approximations for airborne pathogen transmission where spatial and temporal heterogeneities matter, selecting & learning from hybrid CFD if needed

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Typical simplified models

- Computation-reducing assumptions, *e.g.*
  - Well-mixed room
  - Steady state flow
- In many cases suffice
- But there are other of cases in which accuracy is poor:
  - Inadequate mixing; hotspots
  - Rapid changes; transients

Fully-Dynamic Computational Fluid Dynamics (CFD) Model

- Most accurate (with a sufficiently fine or adaptive mesh)
- But may be prohibitively expensive (depending on the scenario and context)

Hybrid (Dynamic/Steady-State) CFD Model

- Divides into different Domains and splices the respective models together.
  - Fully-Dynamic model only where needed
  - Steady-State model everywhere else
- Similar accuracy to pure fully-dynamic CFD
- Much less computationally expensive, however
- But cost still may be prohibitive for many scenarios and contexts

Corrections upon simpler models

- For example, the **Bazant *et al* (2021)** well-mixed room model[1] has two enhancements:
  - Transient
  - Respiratory jet
- In many cases, these simple enhancements may be sufficiently accurate
- But in others, more sophisticated enhancements or models (*e.g.*, hybrid CFD) may be needed….

[1]PNAS April 27, 2021 118 (17) e2018995118; https://doi.org/10.1073/pnas.2018995118

Machine Learning Corrections to simpler models

- We propose using Machine Learning (ML) to produce correction factors that
  - Apply to larger variety and more complex cases
  - Are more accurate than can be obtained by simple corrections (where applicable)
  - Estimate the associated uncertainty in the correction accuracy
  - Determine *which* model should be run if the uncertainty is too high

ML-trained Agent Based Models (ABM)

- ML can also be used in constructing the probabilistic scenarios *via*
  - Training agents on the movements and interactions of actual humans in a space
  - Deploying the agents to extrapolate a fuller range of scenarios than those recorded
  - Deriving the effective Probability Density Function for potential human movements

Model Validation

- The ML-CFD model will be validated against:
  - A reference fully-dynamic CFD model
  - Experimental results: concentration measurements, and/or
  - A real-world scenario by successfully modeling the outcomes