

Viral fate and transport for COVID-19: A high-fidelity Multi-physics Mod/Sim Approach

PRES E NTE D BY

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Computational Thermal and Fluid Mechanics

Sandia National Laboratories SAND-TBD

DOE NASA

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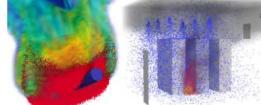
Objectives

- Overview of mass, momentum, energy, and species multi-phase turbulent flow PDE/ODE set
- Discretization, fluids, and Lagrangian coupling
- Confidence demonstrated for unstructured multi-physics turbulent applications
- High Performance Computing drivers
- Established Code Credibility
 - Code verification
 - Model validation
- Uncertainty quantification techniques to deploy
- Case Study:
 - Coughs in open spaces
 - Coughs and breathing (with and without protective shield)
- Possible research paths to explore

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1

3 Proposed Math Model Suite (Eulerian)

• Variable-density low-Mach Eulerian/point-Lagrangian multi-physics coupling
 • Large-eddy simulation-based (low-pass spatial filter); RANS supported, not considered
 • S_k represents coupling from Lagrangian evolution and represents source/sink of mass, momentum, energy, and species

$$\int \frac{\partial \bar{\rho}}{\partial t} dV + \int \bar{\rho} \tilde{u}_j n_j dS = \int S_m dV,$$

$$\int \frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} dV + \int \bar{\rho} \tilde{u}_i \tilde{u}_j n_j dS = \int \tilde{\sigma}_{ij} n_j dS - \int \tau_{ij}^{sgs} n_j dS \quad \sigma_{ij} = 2\mu \tilde{S}_{ij}^* - \bar{P} \delta_{ij},$$

$$+ \int (\bar{\rho} - \rho_o) g_i dV + \int S_{ui} dV \quad \tilde{S}_{ij}^* = \tilde{S}_{ij} - \frac{1}{3} \delta_{ij} \tilde{S}_{kk}$$

$$\int \frac{\partial \bar{\rho} \tilde{\phi}}{\partial t} dV + \int \bar{\rho} \tilde{\phi} \tilde{u}_j n_j dS = - \int \bar{q}_j n_j dS - \int \tau_{\phi,j}^{sgs} n_j dS + \int S_{\phi} dV.$$

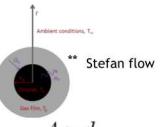
$$\bar{q}_j = - \left[\frac{\mu}{Pr} \frac{\partial h}{\partial x_j} - \frac{\mu}{Pr} \sum_{k=1}^K h_k \frac{\partial Y_k}{\partial x_j} \right] - \frac{\mu}{Sc} \sum_{k=1}^K h_k \frac{\partial Y_k}{\partial x_j}. \quad Le = \frac{Sc}{Pr} = \frac{\alpha}{D}. \quad \bar{q}_j = - \frac{\mu}{\sigma} \frac{\partial \tilde{\phi}}{\partial x_j},$$

$$\tau_{ij}^{sgs} \equiv \bar{\rho} (\tilde{u}_i \tilde{u}_j - \bar{u}_i \bar{u}_j). \quad \tau_{h,j}^{sgs} \equiv \bar{\rho} (\tilde{\phi} \tilde{u}_j - \bar{\phi} \bar{u}_j). \quad \tau_{ij}^{sgs} - \frac{\tau_{kk}^{sgs}}{3} \delta_{ij} = -2\mu^{sgs} \tilde{S}_{ij}^*.$$

Multiple LES models supported...

3

4 Proposed Math Model Suite (point-Lagrangian)



• Spherical Lagrangian droplets

Relaxation time $\tau_p = \frac{4\rho_p d_p}{3\rho_g C_D |\mathbf{u}_g - \mathbf{u}_p|}$.

$$\frac{dx_{p,i}}{dt} = u_{p,i}.$$

Subgrid fluctuations

$$\frac{du_{p,i}}{dt} = \frac{(u_{g,i} - u_{p,i})}{\tau_p} + \left(\frac{\rho_p - \rho_g}{\rho_p} \right) g_i, \quad C_D = 24(1 + Re_p)^{2/3} / Re_p \text{ for } Re_p < 1000.$$

Particle Reynolds number $Re_p = \frac{\rho_g d_p |\mathbf{u}_g - \mathbf{u}_p|}{\mu_g}$ Circa 1950s (Spalding, 1953)

$$C_D = 0.424 \text{ for } Re_p > 1000$$

$$u_p = \frac{d_p^2 (\rho_p - \rho_f) g}{18 \mu_p} \quad B_T = (1 + B_M)^{\frac{Pr}{Sc} \frac{Sc}{Nu}} - 1.$$

$$c_p m_p \frac{dT_p}{dt} = \dot{m} \left(\frac{h_f - h_{f,p}}{B_T} - h_v \right), \quad \text{Spalding heat and mass transfer number}$$

$$B_M = \frac{Y_f - Y_g}{Y_p - Y_f}.$$

Raoult's law and Clausius/Clapeyron (liquid/vapor equilibrium)

$$\hat{N}u = \frac{Nu}{Nu_0} = \left(1 + 0.3 Pr^{\frac{1}{2}} Re_p^{\frac{1}{2}} \right),$$

Ranz-Marshall correlation (1952)

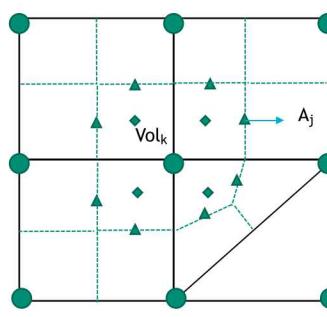
$$\hat{Sh} = \frac{Sh}{Sh_0} = \left(1 + 0.3 Sc^{\frac{1}{2}} Re_p^{\frac{1}{2}} \right).$$

See Fuego manual, or excellent derivation under Wikipedia: https://en.wikipedia.org/wiki/Droplet_vaporization **

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5 Chosen Discretization:
Control-Volume Finite Element Method (CVFEM)

- A combination between the edge-based vertex-centered and FEM is the method known as Control Volume Finite Element (CVFEM) (Hex, Tet, Pyr, Wedge)
- A dual mesh is constructed to obtain flux and volume quadrature locations
- As with FEM, a basis is defined:

$$T(x_k) \approx \sum_{i=1}^{npe} N_i(x_k) T_i \quad \frac{\partial T(x_k)}{\partial x_j} \approx \sum_{i=1}^{npe} \frac{\partial N_i(x_k)}{\partial x_j} T_i$$


- Integration-by-parts over test function w:

$$\int w \rho C_p \frac{\partial T}{\partial t} dV + \int \frac{\partial w}{\partial x_j} \lambda \frac{\partial T}{\partial x_j} dV - \int w \lambda \frac{\partial T}{\partial x_j} n_j dS = 0$$

- However, define a test function, w, as a piecewise constant function (Heaviside) to be 1 inside the dual volume and 0 outside. Gradient is a Dirac-delta function: $\frac{\partial w}{\partial x_j} = -n_j \delta(x_j - x^{IP}_j)$
- Leading to: $\int \rho C_p \frac{\partial T}{\partial t} dV - \int \lambda \frac{\partial T}{\partial x_j} n_j dS = 0$

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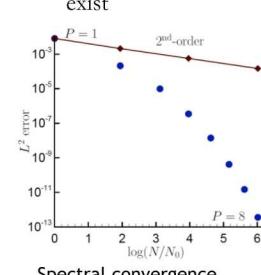
6 Control-Volume Finite Element Method Attributes

- CVFEM can be viewed as Petrov-Galerkin method
- The method can also be promoted in polynomial space, see Domino, *CTRSP*, 2014 as a first example of low-Mach fluids algorithm – or Domino, *JCP*, 2018
- Research Thrust: Possible higher efficiency on NGP due to increased local work)
- However, suitability of higher-order for LES is an open argument – especially when other errors/uncertainties exist



Time: 0.055000
Time: 0.055000

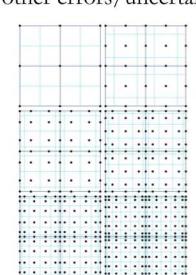
Rotating cube (Re 4000, RPM 3600)
P=1 (top) and P=2 (bottom)



L^2 error

$\log(N/N_0)$

Spectral convergence



Dual-volume for promoted quad4

6

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L^2 error vs $\log(N/N_0)$ for Spectral convergence (P=1 to 8)

Dual-volume for promoted quad4

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P=1 (top) and P=2 (bottom)

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www.elsevier.com/locate/jcp

Design-order, non-conformal low-Mach fluid algorithms using a hybrid CVFEM/DG approach
Stefan P. Domino
Scuola Nazionale Superiore di Studi Avanzati, 1541 P.O. Box 5000-56100, Trieste, Italy
United States

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8 Incremental Approximate Pressure-Projection with Pressure Stabilization Errors

Let the inverse of \mathbf{A} , \mathbf{A}^{-1} be approximated by \mathbf{B}_2 as a scalar, τ (which is \sim time scale)

Let \mathbf{B}_1 be equal to the scaled Laplace operator, $-\tau\mathbf{L}$

Momentum and Continuity: $\begin{bmatrix} A & 0 \\ D & -\tau L \end{bmatrix} \begin{bmatrix} \hat{u} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} \hat{f} \\ -D\tau G p^n \end{bmatrix} \quad \begin{cases} A\hat{u} = f - Gp^n \\ D\hat{u} = \tau(Lp^{n+1} - DGp^n) \end{cases}$

Nodal Projection: $\begin{bmatrix} I & \tau G \\ 0 & I \end{bmatrix} \begin{bmatrix} u^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} \hat{u} \\ \hat{p} \end{bmatrix} + \begin{bmatrix} \tau G p^n \\ 0 \end{bmatrix} \quad \begin{cases} u^{n+1} = \hat{u} - \tau G(p^{n+1} - p^n) \\ p^{n+1} = \hat{p} \end{cases}$

The new splitting and stabilization error is given by:

$$\begin{bmatrix} A & G \\ D & 0 \end{bmatrix} \begin{bmatrix} u^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix} + \begin{bmatrix} (I - A\tau)G(p^{n+1} - p^n) \\ \tau(L - DG)p^{n+1} \end{bmatrix}$$

The above can be shown to hold a second-order temporal error (coming) residual, PSPG

Here, due to equal-order interpolation, i.e., collocation of primitives, $\mathbf{L} \neq \mathbf{DG}$

Therefore, $\mathbf{L} \cdot \mathbf{DG} \sim 4^{\text{th}}$ -order pressure stabilization (pressure oscillations damped)

Therefore, pressure-stabilization error remains

Examples:

- Rhein-Chow (1983)
- Peric (1985)
- Fine-scale momentum

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9 | Coupling Details

- Eulerian solve is fully-implicit (BDF2); Lagrangian solve is explicit
- Multi-stage stiff ODE integrator with exact or approximate (FD-based) Jacobians
- For more gory details on implementation and verification, see the ASC Fuego theory manual: <https://prod-ng.sandia.gov/techlib-noauth/access-control.cgi/2017/1710407.pdf>

Lagrangian Advance (interpolation in time for fluids state)

Stiff ODEs generally drive multiple steps (adaptive; minimum step count specification)

Fluids Solve (allows for disparate mesh resolution)

```
while (pIsActive) {
    integrateInElem();
    faceElemConnect();
    communicate();
} load_balance();
```

Fluids Mesh

Fluids fields

Particle Mesh

Eulerian source terms

Stick/pass/bounce

Droplet trajectory accumulating mass, momentum, energy

9

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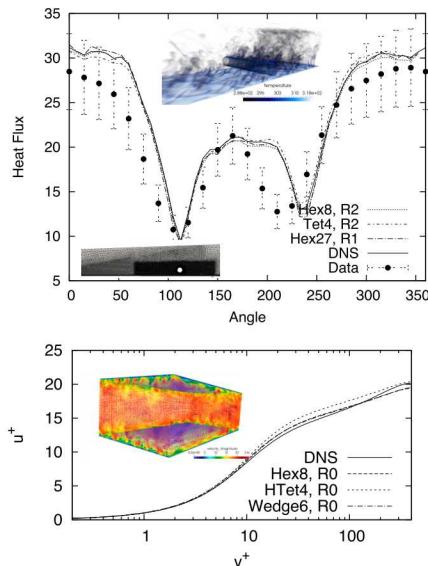
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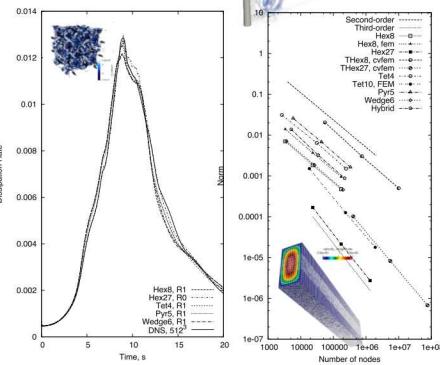
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11 Confidence Established for Atypical Element Topos

Validation



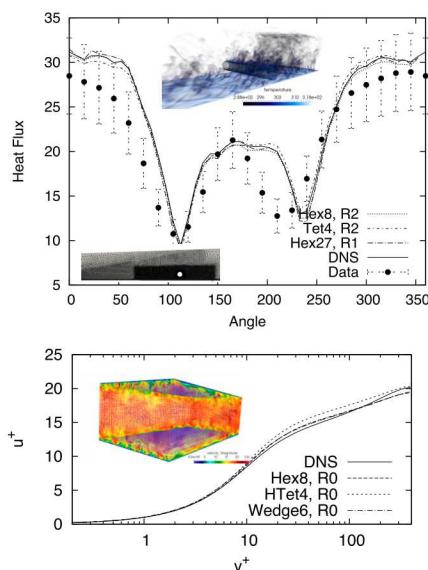
Verification



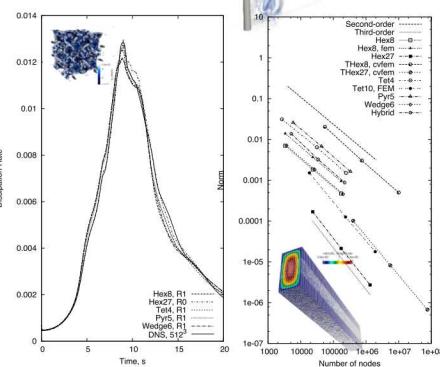
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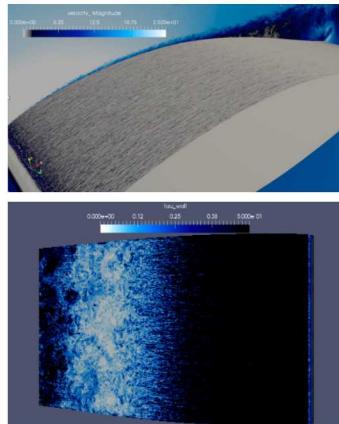
Verification



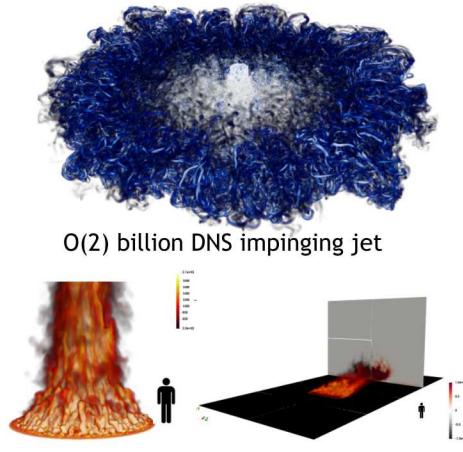
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13 A Note on High Performance Computing

- SNL is committed to High Performance Computing (HPC) to support its science and engineering objectives



O(6) billion wind energy application

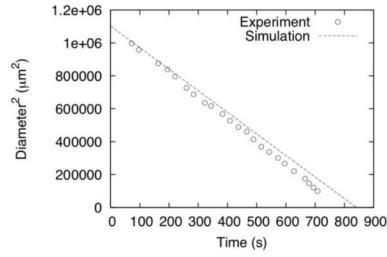
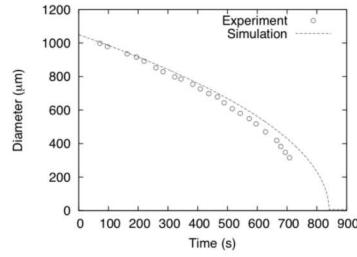
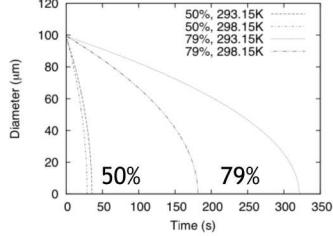
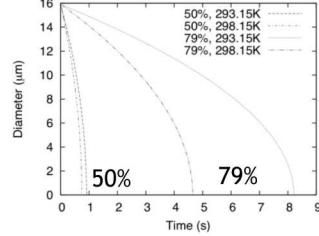


O(200) million multi-physics fire

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14 Established Code Credibility; Evaporation Model Validation

- Ranz and Marshall, 1952 evaporation curves; 0% RH; See Fuego manual for verification

Validation
 D^2 establishedExploration,
 $d = f(RH, T^a)$
Miami vs ABQ

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15 Quiescent Modeling Assumptions: To Include or Not Include: Evaporation and Coupling to Flow Field

- Large droplets ($> 100 \mu\text{m}$), regardless of modeling assumptions, deposit quickly
- High crosswind velocity (10 m/s and higher) can increase deposition distance
- Small droplet nuclei (low-Stokes number) are highly coupled to fluid flow

Conclusions:

- For O(1) scoping simulations, evaporation can probably be neglected
- Droplet transport should always be coupled to carrier fluid (cough, sneeze, breathing); Eulerian source terms (generally) \ll small
- Two-way coupling/droplet tracking is safest, especially since due to low numbers, the cost for droplet tracking is very [very] low

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16 Established Code Credibility; Turbulent Fluid Mechanics

- L. Fan, Turbulent buoyant jets into stratified or flowing ambient fluids, Ph.D. thesis, California Institute of Technology (1967)
- LES is viable *when you can resolve the flow* as models are generally simplistic

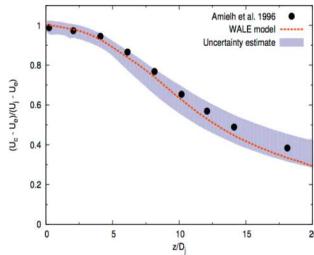
• Baroclinic terms small; Nicolette, Tieszen, Black, and Domino, SAND-20056273
 • Buoyant instabilities low; Kyle and Sreenivasan, JCP 1993

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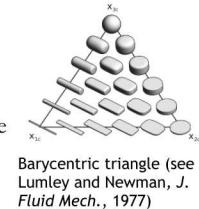
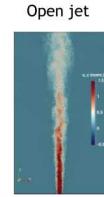
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Improved VVUQ: Automatic Structural Uncertainty

- Most LES validation studies establish structural uncertainty via direct model implementation and forward-calculations
- Is there a more efficient approach? Yes! Eigenvalue perturbation of the SGS stress (extension of RANS-based approach: Emory et al., *Phys. Fluids*, 2017)



$$\begin{aligned}
 \tau_{ij}^{sgs} - \frac{\tau_{kk}^{sgs}}{3} \delta_{ij} &= -2v_{sgs} \bar{S}_{ij}, \\
 a_{ij}^{res} &= \frac{1}{\bar{u}_k \bar{u}_k} \left(\bar{u}_i \bar{u}_j - \frac{\bar{u}_k \bar{u}_k}{3} \delta_{ij} \right) = v_{in}^{res} \Lambda_{nl}^{res} v_{jl}^{res} \\
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 \bar{u}_i \bar{u}_j^* &= \bar{u}_i \bar{u}_j + \tau_{ij}^{sgs*} = \bar{u}_i \bar{u}_j + \bar{u}_k \bar{u}_k^* a_{ij}^{sgs*} + \frac{\tau_{kk}^{sgs*}}{3} \delta_{ij}, \\
 \text{with } \bar{u}_k \bar{u}_k^* &= \bar{u}_k \bar{u}_k + \tau_{kk}^{sgs*} \quad \text{and} \quad a_{ij}^{sgs*} = v_{in}^{sgs*} \Lambda_{nl}^{sgs*} v_{jl}^{sgs*}.
 \end{aligned}$$

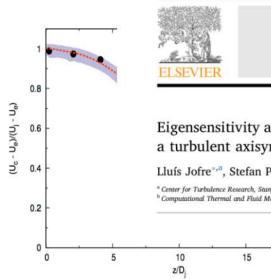
Barycentric triangle (see Lumley and Newman, *J. Fluid Mech.*, 1977)

17

18

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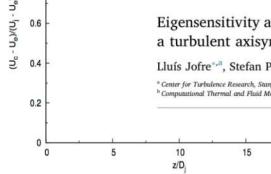


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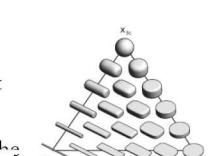
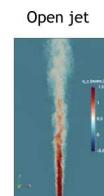
Eigensensitivity analysis of subgrid-scale stresses in large-eddy simulation of a turbulent axisymmetric jet

Lluís Jofre^a, Stefan P. Domino^b, Gianluca Iaccarino^a^a Center for Turbulence Research, Stanford University, Stanford, CA 94305, USA^b Computational Thermal and Fluid Mech.

Flow Turbulence Combust (2018) 100:341–363

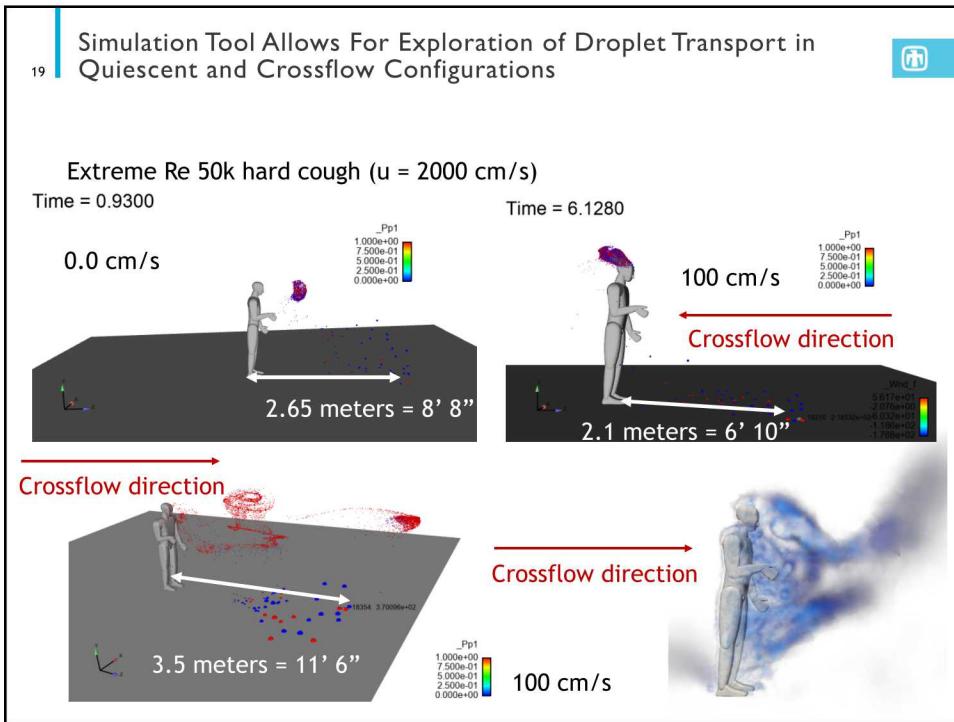
DOI 10.1007/s10494-017-9844-8

A Framework for Characterizing Structural Uncertainty in Large-Eddy Simulation Closures

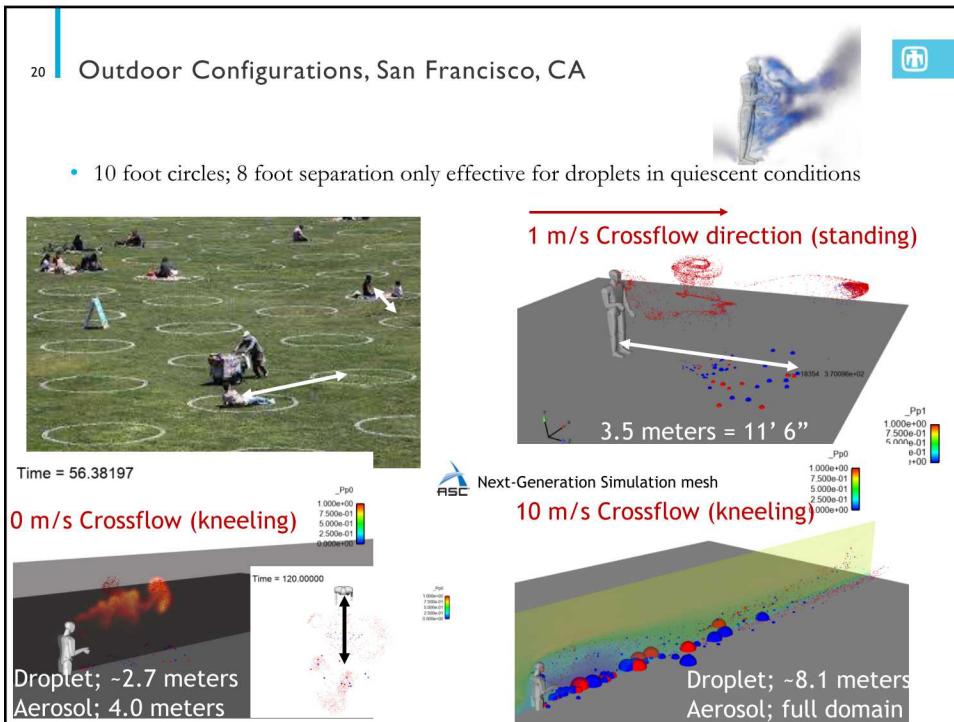
Lluís Jofre¹ · Stefan P. Domino² · Gianluca Iaccarino¹Barycentric triangle (see Lumley and Newman, *J. Fluid Mech.*, 1977)

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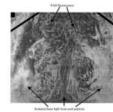
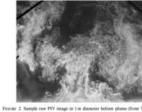
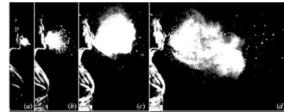
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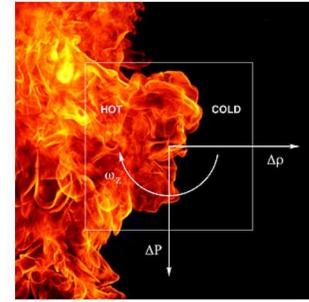
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Investment in a Validation Dataset is Suggested



Current experiments are macroscopic (vs.... PIV, PLIF) O'Hern et al., JFM, 2005 Tieszen et al., C&F 2002

Lack of good finite-pulsed jet data



Thankfully, this application does not note substantial turbulent kinetic energy production via a baroclinic mechanism (small density ratio, At# ~0.0)

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Conclusions

- Model Suite includes coupling between Eulerian and Lagrangian regions
- Mass, momentum, energy, species multi-phase turbulent flow
- Verification and Validation pedigree established for numerics/models
- Credibility established for evaporating physics and buoyant jets
- High-performance computing is a routine requirement

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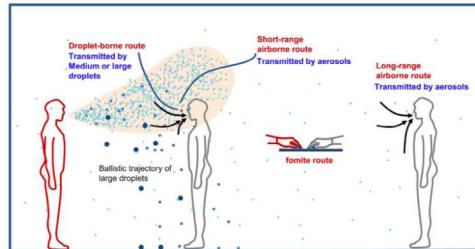
23 Extra

- Full talk includes more details

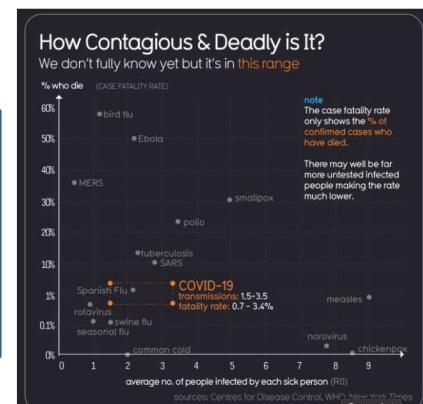
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24 Pathogen Transport and Infection Mechanisms

- Direct and Indirect transmission mechanism



Wei and Li, A. J. Infect. Cont., 2016



Informationisbeautiful.net

- **Caveat:** currently, the open news cycle is not distinguishing between fluid mechanics transport of droplets emanating from a cough/sneeze and the likelihood of infection by either direct or indirect transmission
- As fluid mechanists, we can provide leadership towards answering the former while partnering with those who can speak towards pathogen viability and infection mechanism by providing detailed time-history trajectories

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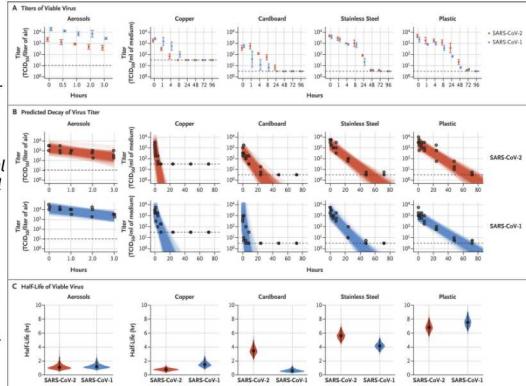
Viability of SARS-CoV-2 Aerosols

- Morris et al, "Aerosol and Surface Stability of SARS-CoV-2 as Compared with SARS-CoV-1", New England Journal of Medicine, April 16, 2020.

The half-lives of SARS-CoV-2 and SARS-CoV-1 were similar in aerosols, with median estimates of approximately 1.1 to 1.2 hours and 95% credible intervals of 0.64 to 2.64 for SARS-CoV-2 and 0.78 to 2.43 for SARS-CoV-1

We found that the stability of SARS-CoV-2 was similar to that of SARS-CoV-1 under the experimental circumstances tested. This indicates that differences in the epidemiologic characteristics of these viruses probably arise from other factors, including high viral loads in the upper respiratory tract and the potential for persons infected with SARS-CoV-2 to shed and transmit the virus while asymptomatic.³⁴

Our results indicate that aerosol and fomite transmission of SARS-CoV-2 is plausible, since the virus can remain viable and infectious in aerosols for hours and on surfaces up to days (depending on the inoculum shed). These findings echo those with SARS-CoV-1, in which these forms of transmission were associated with nosocomial spread and super-spreading events,³⁵ and they provide information for pandemic mitigation efforts.



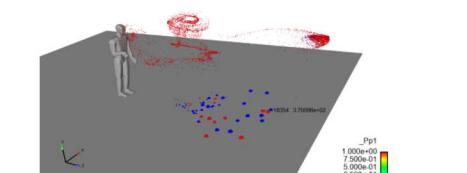
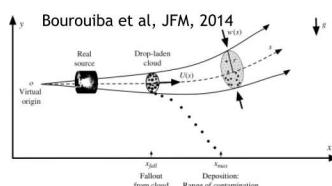
Excerpt from Morris et al., 2020

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Modeling droplet dispersion from human coughs and sneezes in complex environments

- Objective: Deploy multi-physics mod/sim capability to understand droplet deposition and pathogen transport originating from human coughs to understand airborne transmission and surface contamination of COVID-19 in common public spaces



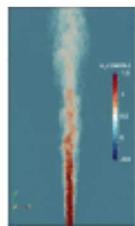
Fuego synthetic cough simulation with droplet distribution from Yang et al, J. Aerosol Med, 2007 including pathogen probability

- Coughs are turbulent buoyant, multiphase plumes (Re~25K for coughs)
- Large droplets deposit while small droplets persist
- Evaporation rates, which are environment-specific, provides understanding towards what droplets deposit and those that persist
- Droplet nuclei can persist in the environment and *may* pose a long term risk to occupants

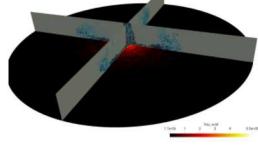
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27 Why Sandia?

- Thermal/Fluids Core Competency rests in turbulent, buoyant, multi-phase transport

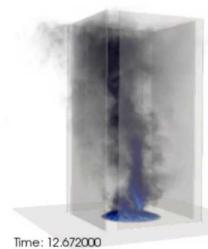


Time: 0.346813



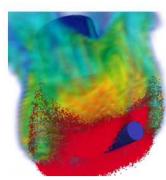
Turbulent jets

R1, 20cm

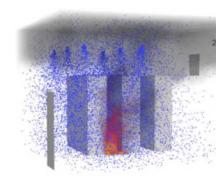


Time: 12.672000

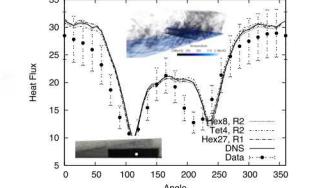
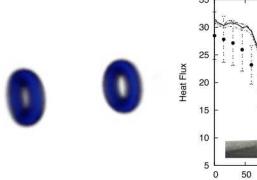
- Jofre, Domino, and Iaccarino, IJHT, 2019
- Domino, Sakiavich, Barone, Comp&F 2019
- Domino, JCP 2018



Deposition and suppression



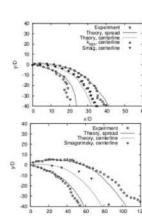
Vortex dynamics



Quality unstructured numerics

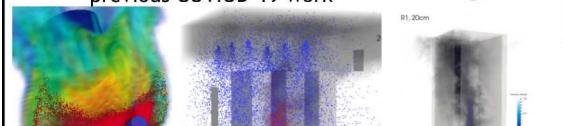
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28 Primary Objective: Establish a Credible High-Fidelity Multi-physics Tool

Figure 4: Froude 10 and 40 validation results and volume-rendered mixture fraction. Data manually extracted from [\[4\]](#)

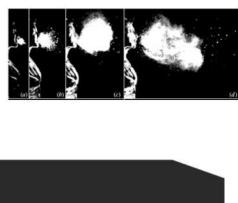
Validation for droplet evaporation Ranz & Marshall, 1952;
Hamey, 1982 and plume dynamics Fan, 1967

- Goal: Close the credibility gaps from previous COVID-19 work

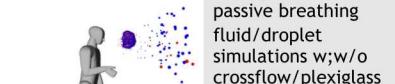


Deploy multi-physics code capability: Sierra/Fuego low-Mach turbulent reacting flow code with point-Lagrangian coupling

Time = 0.0600

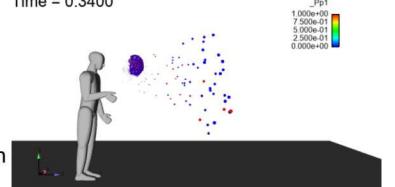


Time = 0.2000



Multi-physics coughs
passive breathing
fluid/droplet
simulations w/w/o
crossflow/plexiglass

Time = 0.3400



28

29 | Droplet Size Distribution; Settling Speed; Physics Description

- Size, number and cough velocity are well characterized starting from as early as 1946
- Uncertainty in the literature

FIGURE 17. (Colour online) Histogram of droplet size in coughs (reproduced from Duguid 1946).

• Settling Speed:

$$m_p \frac{du_p}{dt} = \frac{m_p (u_p - u_f)}{\tau_p} + (m_p - m_f)g$$

$$u_p = \frac{d_p^2 (\rho_p - \rho_f)g}{18\mu_p}$$

Figures/Images again provided by Bourouiba et al, JFM, 2014

• Buoyancy, which affects plume dynamics, are known to be significant factors

FIGURE 5. (Colour online) (a) The effect of buoyancy on the sneeze cloud is apparent in its upward curvature. (b) The large droplet trajectories are shown in the streak image recorded at 2000 f.p.s.

Modest room ventilation can easily suspend a droplet nuclei

Droplet Size (μm)	Settling Velocity (cm/s)	Settling Time for 2m height (s)	Evaporation Time (s)
100	~30	~6.6	~7
1	~3e-3	~66e3 (18.5 hr)	~7e-4

29

30 | Findings: a) Droplet Nuclei Clustering/Persistence, b) Protective Shrouds are Effective for Primary Deposition Mitigation

Top wall not shown

Time = 0.0735 second: Time = 1.0352 second: Time = 8.0071 second: Time = 120.0000 seconds

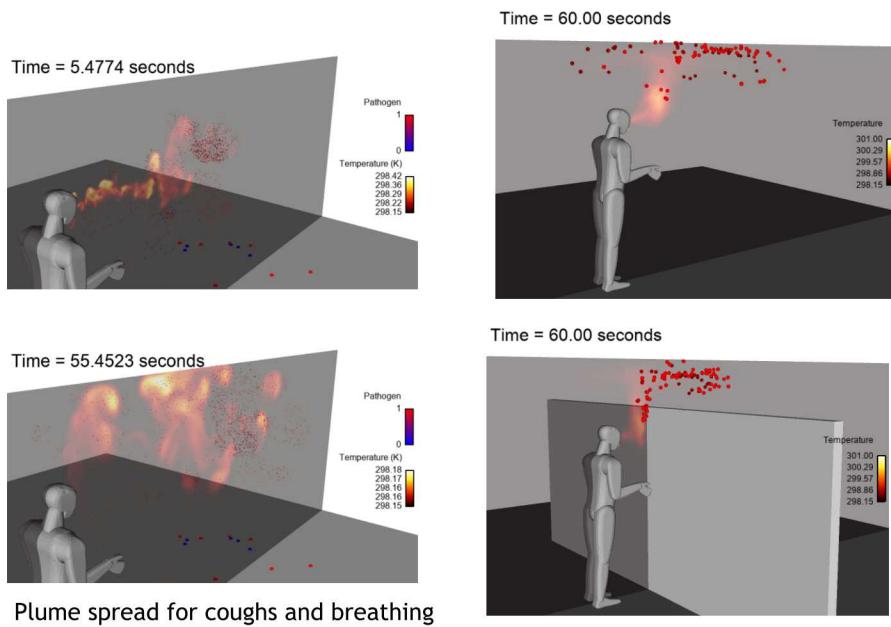
Pulsed nominal cough jet with (Top) and without (Bottom) protective shroud; R2 mesh

Time = 0.0736 second: Time = 0.4815 second: Time = 8.0782 second: Time = 120.0000 seconds

30

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Findings: a) Droplet Nuclei Clustering/Persistence, b) Protective Shrouds are Effective for Primary Deposition Mitigation



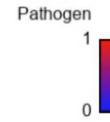
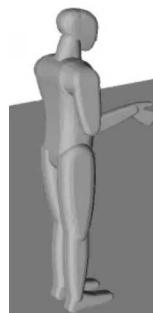
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Findings: a) Droplet Nuclei Clustering/Persistence, b) Protective Shrouds are Effective for Primary Deposition

Time = 0.0000 seconds

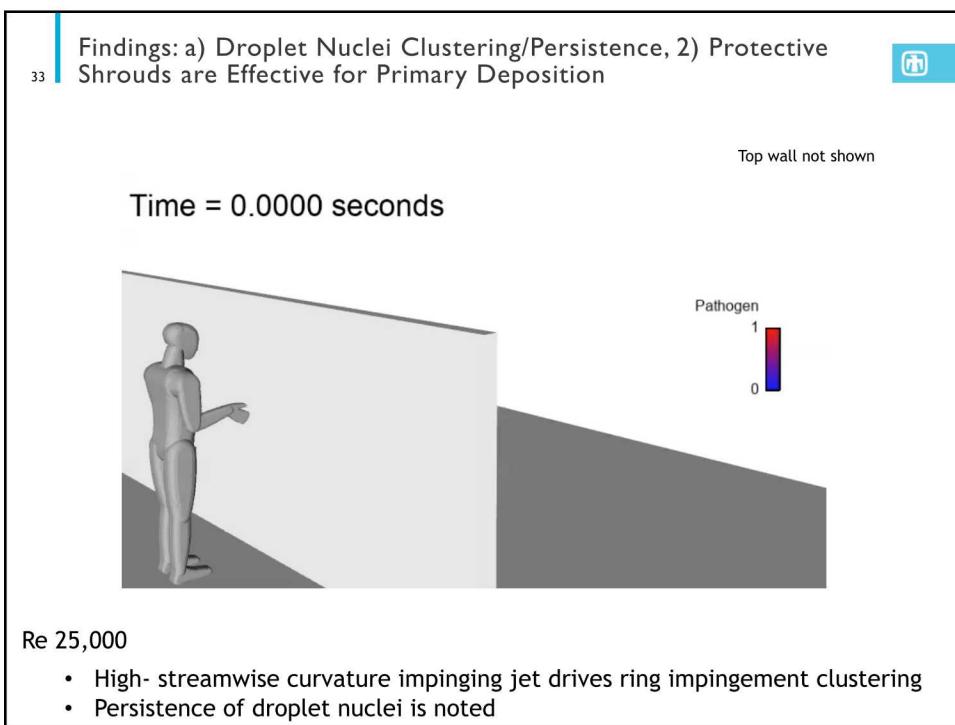
Top wall not shown



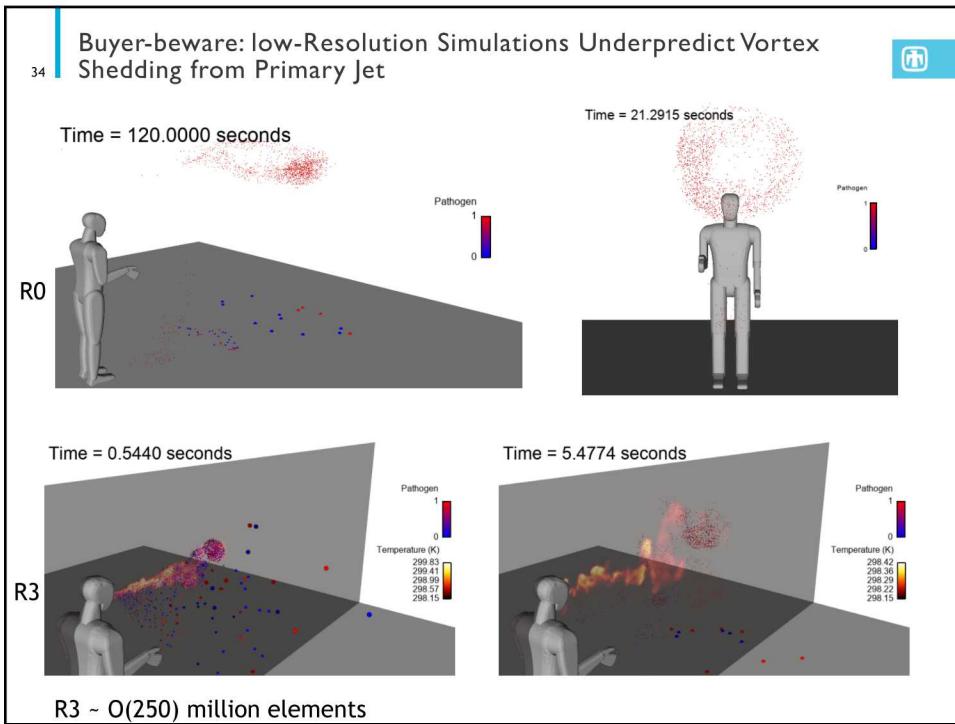
Re 25,000

- Classic axisymmetric jet shedding drives droplet clustering
- Primary droplet cloud in addition to secondary buoyant plumes

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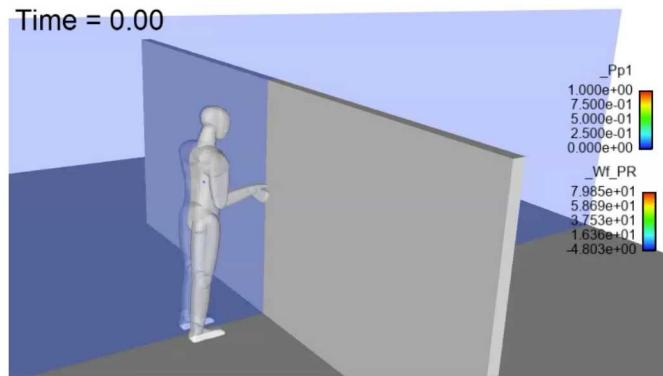


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The Role of Protective Shrouds; Passive Breathing in Zero crossflow

Wan et. al, Particle Size Concentration Distribution and Influences on Exhaled Breath Particles in Mechanically Ventilated Patients; 2014



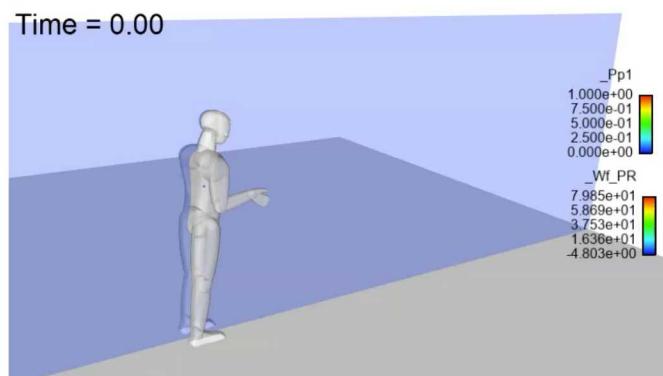
- 1, 2, and 3 micron spray distribution; $120e-12$ g injection over 4 seconds; sinusoidal breath of 100 cm/s
- Low velocity and small droplets render direct transmission unlikely, however, as with previous simulations, droplet nuclei persist - now at low concentrations

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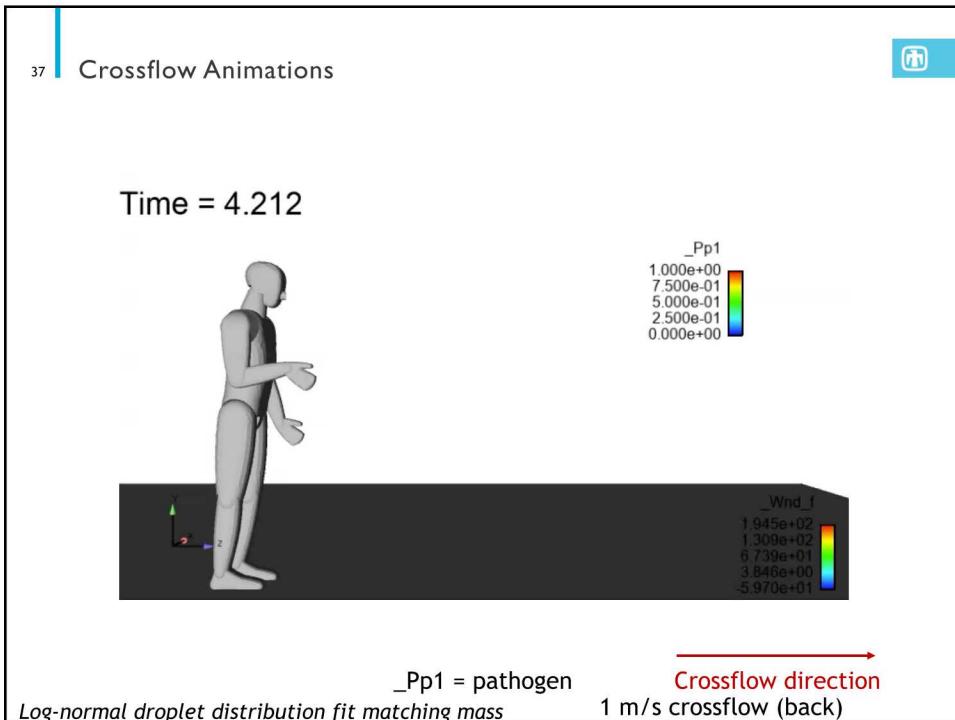
The Role of Protective Shrouds; Passive Breathing in Zero crossflow

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