Detailed Simulation of Viral Propagation and Mitigation in the Built Environment

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Outline

- Pathogen Transmission
- Mitigation Options
- Physical Modeling
- Numerical Methods
- Examples
- Reopening After the Crisis
- Conclusions and Outlook

Pathogen Transmission

Virus Transmission: Sneezing



Virus Transmission: Breathing



Virus Transmission: HVAC/Wakes



Virus Transmission

- Entering the Body: Nose, Mouth, Eyes
- Exiting the Body: Nose, Mouth
 - Sneeze, Cough, Shout, Sing, Speak, ...
- → Transmission Modes:
 - Person-to-Person
 - Person-Air-Person
 - Person-Surface-Person

- : Large/Small Droplets
- : Small Droplets
- : Large Droplets

Droplet Distribution When Coughing



R.G. Loudon and R.M. Roberts - Droplet Expulsion from the Respiratory Tract; Am. Rev. Respir. Dis. 95, 3, 435–442 (1967).

Sink Velocities of Droplets in Air

Diameter [mm]	Sink Velocity [m/sec]	Reynolds-Nr.
1.0e+00	3.01e+01	1.99e+03
1.0e-01	3.01e-01	1.99e+00
1.0e-02	3.01e-03	1.99e-03
1.0e-03	3.01e-05	1.99e-06
1.0e-04	3.01e-07	1.99e-09

Droplet Evaporation



X. Xie, Y. Li, A.T.Y. Chwang, P.L. Ho, W.H. Seto - How Far Droplets Can Move in Indoor Environments – Revisiting the Wells Evaporation-Falling Curve; Indoor Air 17, 211-225 (2007). doi:10.1111/j.1600-0668.2006.00469.x

Viral Load / Infectious Dose

- Many Factors:
 - State of Immune Defenses of Victim
 - Timing of Viral Entry (All at Once, Piece by Piece)
 - Hair and Mucous in Nasal Vessels,
- Data From Biological Warfare Agents [Fra97]

– Brucellosis	10-100
– Q fever	1-10
- Tularaemia	10-50
 Smallpox 	10-100
– Viral Haemorrhagic Fevers	1-10
– Tuberculosis	1 (!!)

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– Brucellosis	10-100	
– Q fever	1-10	Cov-19: 100-200
– Tularaemia	10-50	
 Smallpox 	10-100	
 Viral Haemorrhagic Fevers 	1-10	
– Tuberculosis	1 (!!)	

Covid-19 Lifetime Outside the Body

- Air: 1-2 Hours
- Some Surfaces: 1-2 Days
- Some Variability With Humidity/Temperature
- Some Variability With UV/Sunlight Radiation
 The More Sunlight, The Shorter The Lifetime

Infectivity of Covid-19

https://tinyurl.com/FAQ-aerosols



Figure: relative probability of transmission of SARS-CoV-2 from an infected individual as a function of time in the disease. The peak of infectiveness is just before the onset of symptoms. Reference: <u>Prof. A Marm</u> <u>Kilpatrick</u>, University of California-Santa Cruz.

Infectivity of Covid-19

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Covid-19 vs. Influenza/Flu

- Max Yearly US Deaths From Influenza/Flu: 60K
 No Lockdowns, No Preventive Measures
- US Deaths After 12-Months of Covid-19: 400K
 With Lockdowns, With Preventive Measures

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 No Lockdowns, No Preventive Measures
- US Deaths After 12-Months of Covid-19: 400K
 With Lockdowns, With Preventive Measures
- → Covid-19 Orders of Magnitude More Deadly Than Influenza/Flu

Mitigation Options

Mitigation of Virus Transmission

- 2 Main Modes:
 - Large Droplets \rightarrow `Spitting'
 - Small Droplets → `Smoke'

Procedure Measure	Large Droplets (spitting)	Small Droplets (cigarette smoke)	Person-Air- Person	Person-Surface- Person
2m/6ft Distance				
Face Masks				
Periodic Hand Cleaning		X		
Plexiglass Shields				
1-Way Person Traffic				
2x Daily Cleaning				
Nightly UV Cleaning				
Maximize Fresh Air in HVAC	X			X
Hard UV Lamps in HVAC Ducts	X			X
HEPA Filters in HVAC Ducts	X			X
Upper Room UV Cleaning	X			X

Physics

Air: Navier-Stokes, Incompressible

Conservation of Mass, Momentum and Energy:

$$\nabla \cdot \mathbf{v} = 0$$

$$\rho \mathbf{v}_{,t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla p = \nabla \mu \nabla \mathbf{v} + \rho \mathbf{g} \beta (T_0 - T) + \mathbf{f}$$

$$\rho c_p T_{,t} + \rho c_p \mathbf{v} \cdot \nabla T = \nabla k \nabla T + \mathbf{s}$$

ρ: Density **v**: Velocity *ρ*: Pressure *μ*: Viscosity

g: Gravity

T: Temperature

- c_p : Heat Capacitance
- k: Thermal Conductivity
- β : Expansion Coefficient
- f,s: External Forces/Heat Sources

Equations for Diagnostics

Age of Air

$$a_{,t} + \mathbf{v} \cdot \nabla a = 1$$

• Pathogen Concentration

$$c_{,t} + \mathbf{v} \cdot \mathbf{V}c = \mathbf{V}d_c\mathbf{V}c + \mathbf{s}_c$$

UV Irradiation

$$I_{,t} + \mathbf{v} \cdot \nabla I = \nabla d_I \nabla I + \mathbf{s}_{\mathrm{I}}$$

Particle Motion and Temperature

• Velocity and Position

$$\rho_p \frac{\pi d^3}{6} \frac{d\mathbf{v}_p}{dt} = \mathbf{D} \quad ; \quad \frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p$$

• Temperature

$$\rho_p c_{pp} \frac{\pi d^3}{6} \frac{dT_p}{dt} = Q$$

Momentum Transfer

Drag Force of Each Particle

$$D_{i} = \frac{\pi d^{2}}{4} c_{d} \frac{1}{2} \rho |\mathbf{v} - \mathbf{v}_{p}| (\mathbf{v}_{i} - \mathbf{v}_{pi})$$

• Drag Coefficient and Reynolds-Number $c_d = \max\left(0.1, \frac{24}{\text{Re}}\left(1+0.15 \text{Re}^{0.687}\right)\right)$; $\text{Re} = \frac{\rho |\mathbf{v} - \mathbf{v}_p| d}{\mu}$

Heat Transfer

• Heat Flux For Each Particle

$$Q = \pi d^2 \left[h \left(T - T_p \right) + \sigma^{\times} \left(T^4 - T_p^4 \right) \right]$$

• Film Coefficient, Nusselt- and Prandtl-Number

$$h = \frac{k \cdot Nu}{d}$$
; $Nu = 2 + 0.459 \,\mathrm{Pr}^{0.333} \,\mathrm{Re}^{0.55};$ $\mathrm{Pr} = \frac{c_p k}{\mu}$

Numerics

Basic Elements of Solver (1)

- Spatial Discretization: Unstructured Grids
 - Arbitrary Geometries
 - Adaptive Refinement
- Spatial Discretization: Simple FEM
 - One-Type Element Code: Speed and Simplicity
 - Use Tetrahedra Even in Boundary Layers
- Temporal Discretization: Explicit Advection
 - Physically Interesting Scales → Need Accuracy
 - 1-Step Schemes: Moving Grids, Adaptive Refine/Remesh
- Temporal Discretization: Implicit Viscous/Pressure
 - Low-Storage Iterative Solvers

Basic Elements of Solver (2)

- Steady Results: Independent of Timestep
 - Confidence
 - Convergence Study Possible
- Edge-Based Data Structures
 - Reduction of Indirect Addressing
 - Reduction in Flops
- Extensive Renumbering
 - Avoidance of Cache-Misses
 - Shared-Memory Parallel Machines
- Preconditioning:
 - Diagonal: Isotropic Grid
 - Linelets: Stretched (RANS) Grid

Temporal Discretization: Δ-Scheme (1)

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \Delta \mathbf{v}^a + \Delta \mathbf{v}^p = \mathbf{v}^* + \Delta \mathbf{v}^p$$

- Advective / Diffusive Prediction: $v^n \to v^*$ $\left[\frac{1}{\Delta t} - \theta \nabla \mu \nabla\right] (v^* - v^n) + v^n \cdot \nabla v^n + \nabla p^n = \nabla \mu \nabla v^n$
- Pressure Correction: $p^n \rightarrow p^{n+1}$

$$\nabla \cdot \mathbf{v}^{n+1} = 0$$

$$\frac{\mathbf{v}^{n+1} - \mathbf{v}^*}{\Delta t} + \nabla (p^{n+1} - p^n) = 0$$

$$\Rightarrow \Rightarrow \quad \nabla^2 (p^{n+1} - p^n) = \frac{\nabla \cdot \mathbf{v}^*}{\Delta t}$$

Temporal Discretization: Δ-Scheme (2)

• Velocity Correction: $v^* \rightarrow v^{n+1}$

$$\mathbf{v}^{n+1} = \mathbf{v}^* - \Delta t \nabla (p^{n+1} - p^n)$$

Remarks:

- Residuals of Pressure Correction Vanish for Steady-State
 - → Results Not Depend on Projection Scheme
 - → Results Not Depend on Δt

Particle Motion and Temperature

• Position, Velocity and Temperature: ODEs of Type

$$\frac{du}{dt} = r(\mathbf{x}, \mathbf{u}_f, u, t)$$

 Integrated Explicitly; Typically: 4th Order Runge-Kutta

$$u^{n+i} - u^{n+i-1} = \alpha_i \Delta t \cdot r(\mathbf{x}, \mathbf{u}_f, u^{n+i-1}, t^{n+i-1})$$
$$\alpha_i = \frac{1}{k-i+1}$$

Particle Tracking

- Need: Flow Variables At Location of Particle
- → Need Host Element for Each Particle



- Initialization: Bins + Near-Neighbour Search
- Incremental: Near-Neighbour Search
 - Vectorized and Parallelized for OMP
 - Also Running in MPI

UV Radiation

• Irradiation Function of Distance/Angle

1

$$S_I \sim \frac{1}{r^2}$$

- Shading Possible → Ray-Tracing
 - From Element (Gauss-Points) to UV Lamp

Raytracing With FEM Grids

- Any Point P: $\mathbf{x}_{P} = \mathbf{x}_{A} + \mathbf{x}_{BA} \,\xi + \mathbf{x}_{CA} \,\eta + \mathbf{x}_{DA} \,\zeta = \mathbf{x}_{A} + \mathbf{G} \,\xi$ • $\mathbf{a} \xi = \mathbf{G}^{-1} \mathbf{x}_{PA}$
- Given Input Location, Obtain Output $\boldsymbol{\xi} o = \boldsymbol{\xi} i + \mathbf{G}^{-1} \Delta \mathbf{x} = \boldsymbol{\xi} i + \mathbf{G}^{-1} \mathbf{v} \Delta t = \boldsymbol{\xi} i + \boldsymbol{\alpha} \Delta t$
- Output Faces: $\xi_0=0$
- Get min(Δt_i), $\Delta t_i > 0 \rightarrow Neighbour Element$

J. Favre and R. Löhner – Ray Tracing With a Space-Filling Finite Element Mesh; IJNME 37, 3571-3580 (1994)

В
Ceiling UV In Hospital Room



Coupling of CFD and CCD



$CCD \rightarrow CFD$

- Several Options Possible
- Body Fitted
 - Transcribe Discrete Surface from CCD \rightarrow CFD / Merge
 - Move/Smooth/Remesh CFD Mesh
- Embedded
 - Transcribe Discrete Surface from CCD \rightarrow CFD
 - Obtain Intersections With Edges/New BC
- Immersed
 - Transcribe Discrete Volume from CCD \rightarrow CFD
 - Obtain CFD Points Inside CCD Domain/New BC

$\mathsf{CCD} \to \mathsf{CFD}$



Immersed Bodies

Immersed Body: Options

- Desired: In Body Region: v_f = w_b
- **Kinematic**: Impose: $v_f = w_b$
- **Kinetic** : Use Force: $f = c_0 (v_f w_b)$ [Goldstein]
- Kinetic/Kinematic: [Mohd-Yusof]:

$$\mathbf{M}\frac{\Delta \mathbf{v}_i}{\Delta t} = \mathbf{r}_i + \mathbf{f}_i \qquad \Rightarrow \qquad \mathbf{f}_i = \mathbf{M}\frac{\mathbf{w}_i^{n+1} - \mathbf{v}_i^n}{\Delta t} - \mathbf{r}_i$$



Immersed Body: Extensions

- Kinematic:
 - Extend to Higher Order [Balaras]
 - Same as for Embedded
- Kinetic:
 - Use Lagrange Multipliers [Glowinsky]

Search for Points in Bodies: Options

- Option 1:
 - Store CFD Points in Bin/Octree
 - Loop Over Immersed Body Elements
 - Get Bounding Box
 - Get CFD Points in Bounding Box
 - Detailed In/Out Analysis
- Option 2:
 - Store Immersed Body Elements in Bin/Octree
 - Loop Over CFD Points
 - Get Immersed Body Element in Region
 - Detailed In/Out Analysis

Pedestrian Motion

Discrete Models

- Any Pedestrian Flow Simulation:
 - Global Movement: Strategic, Tactical
 - Local Movement: Operational
- Global Movement
 - Targets (Regions/Lines/…) → Will Force
- Local Movement
 - Collision Avoidance
 - Social Force/ Contact Models
 - Local Geometry Info
 - Walls, Paths, Roughness, ...

PEDESTRIAN MOTION

• Newton's Law:

```
\mathbf{m} \mathbf{v}, \mathbf{t} = \mathbf{f}
\mathbf{x}, \mathbf{t} = \mathbf{v}
```

- m: Mass
- v: Velocity
- **x**: Position
- f: Sum of All Forces
- Modeling Effort: f

PEDESTRIAN FORCES

- Internal Forces
 - Will Force (Get There (in Time))
 - Pedestrian Collision Avoidance Forces: Intermediate Range
 - Pedestrian Collision Avoidance Forces : Near Range
 - Wall/Obstacle (Collision) Avoidance Forces
- External Forces
 - Contact: Other Pedestrians
 - Contact: Walls/Obstacles

PEDFLOW

- Mixture of Agent-Based and Social Force Model
- Forces Via by Minimal Set of Well-Defined Parameters
 - Relaxation Time (Fitness)
 - Desired Velocity
 - Pushiness (Distraction)
- Strategic and Tactical: Desired Locations/Time
- Operational: Local Collision Avoidance
- Background Grid for Geometry/Spatial Search
- Edge-Based Data Structures for Pedestrians

R. Löhner – On The Modeling of Pedestrian Motion; Appl. Math. Mod. 34, 2, 366-382 (2010).

Madrid Metro Station

- 3/11/2004 Attack
- Did Blast Analysis
- Follow-Up



Madrid Bomb Attack



Madrid Bomb Attack



Madrid Bomb Attack



Evacuation from Medina Mosque

- Over 10⁵ Pedestrians
- Run on Laptop



Rendering via 3-D Studio Max



Examples

Examples (1)

- Physics and Numerics: FEFLO
- Flow Initialization:
 - Ambient: Quiescent, 20°C
 - Sneeze: Spherical Region, r=5cm, Near Mouth
 - -V=5f(t) [m/sec] ; T=20+(37-20)f(t) [°C]
- Particle Initialization
 - 4 Size Groups; Released Every 0.005 sec for 0.1 sec
 - V=5 m/sec ; T=37°C

f(t)

Examples (2)

- 3 Different Timescales, Depending on Size
 - O(10⁰) sec: Fast, Ballistic Drop of Large d=1.0 mm Particles
 - O(10¹) sec: Slower Drop of Intermediate d=0.1 mm Particles
 - O(10²) sec: Transport of Small d<0.01 mm Particles Through Air
- HVAC Systems:
 - Good Mixers
 - Complex Flowfields
 - \rightarrow Condusive to Pathogen Transmission

Sneezing in TSA Queues



12.47 Mels

Sneezing in TSA Queues



Sneezing in TSA Queues



Sneezing in Hospital Room



Sneezing in Hospital Room



Hospital Room With UV Lamp



Hospital Room With UV Lamp



Sneezing in a Generic Classroom



Sneezing in a Generic Classroom



Sneezing in a Generic Classroom



Classroom With Ceiling-UV



NBC Universal Today Show, September 30 (2020), see: https://www.today.com/health/ventilationcovid-19-reduce-spread-proper-airflow-t192366

Sneezing in Subway



Sneezing in Subway


Sneezing in Subway



M. Gröndahl, Ch. Goldbaum and J. White - What Happens to Viral Particles on the Subway; *New York Times*, August 10 (2020);



Narrow Corridor



Narrow Corridor



Narrow Corridor: Viral Load



Reopening After the Crisis

Reopening After the Crisis

- Will Have/Need Sensors to Monitor Environment
- Basic Questions:
 - How Many ?
 - Placed Where ?
- Current Approach:
 - Run Many Scenarios Cases
 - Place Many Sensors
 - Keep (Recursively) the One Detecting the Most Cases



Hospital Room: Average Velocities



Case Study: Hospital Room

- Cases 1,2,3:
 - Contaminant/Pathogens Through Each of the 3 Different Entry Vents
 - 0-60 sec
- Case 4:
 - Virus Production from Patient
 - 0-10 sec
- Run for 300 sec (5 min) of Real Time
- Measure Contaminant/Pathogen Concentration on all Walls



Max Values Measured During 5 Mins









Wall Data Recorded

- Points With No Cases Measured: 4308
- Points With 1 Case (Out of 4) Measured: 3377
- Points With 2 Cases (Out of 4) Measured: 1010
- Points With 3 Cases (Out of 4) Measured:
- Points With 4 Cases (Out of 4) Measured:
- Excluded Location:
 - Above zmin (Minimum Height Requirement)
 - Not on Beds/Furniture/Patient/Attendant

()

Result: 2 (Optimal) Sensors



Conclusions

- Summarized:
 - Mechanical Characteristics of Virus Contaminants
 - Transmission Via Droplets and Aerosols
- Emphasis on High-Fidelity (Hi-Fi) Physics
 - PDEs
 - Appropriate Numerical Methods
- Examples from the Built Environment
 - TSA Queues, Hospital Rooms, Corridors, Trains, ...
- Optimal Placement of Sensors

Outlook

- Increase Realism
 - Boundary Conditions for HVAC Systems [Entry, Mixing, ...]
- Streamlining Simulation Toolbox/Workflow
- Field These Tools To Enable Smooth Post-Pandemic Transition

Thank You Very Much for Your Attention

Additional Material

Temporal Discretization: Δ-Scheme (1)

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \Delta \mathbf{v}^a + \Delta \mathbf{v}^p = \mathbf{v}^* + \Delta \mathbf{v}^p$$

- Advective / Diffusive Prediction: $v^n \to v^*$ $\left[\frac{1}{\Delta t} - \theta \nabla \mu \nabla\right] (v^* - v^n) + v^n \cdot \nabla v^n + \nabla p^n = \nabla \mu \nabla v^n$
- Pressure Correction: $p^n \rightarrow p^{n+1}$

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Temporal Discretization: Δ-Scheme (2)

• Velocity Correction: $v^* \rightarrow v^{n+1}$

$$\mathbf{v}^{n+1} = \mathbf{v}^* - \Delta t \nabla (p^{n+1} - p^n)$$

Remarks:

- Residuals of Pressure Correction Vanish for Steady-State
 - → Results Not Depend on Projection Scheme
 - → Results Not Depend on Δt

Spatial Discretization: Advection (1)

• Galerkin:

$$\mathbf{r}^{i} = D^{ij}\mathbf{F}_{ij} = D^{ij}(\mathbf{f}_{i} + \mathbf{f}_{j})$$

$$\mathbf{f}_{i} = S^{ij}_{\ k}F_{i}^{\ k} , \quad S^{ij}_{\ k} = \frac{d_{k}^{ij}}{D^{ij}} , \quad D^{ij} = \sqrt{d_{k}^{ij}d_{k}^{ij}}$$

$$d_{k}^{ij} = \frac{1}{2}\int \left(N_{,k}^{i}N^{j} - N_{,k}^{j}N^{i}\right) d\Omega$$

$$\mathbf{f}_{i} = \left(S_{k}^{ij}\mathbf{v}_{i}^{k}\right)\mathbf{v}_{i}$$

Spatial Discretization: Advection (2)

- Need Consistent Numerical Fluxes
 - Integration Along Characteristics
 - Taylor-Galerkin/Streamline Diffusion/SUPG/GLS/...
 - Edge-Based Upwinding
- Consistent Numerical Flux

$$\mathbf{F}_{ij} = \mathbf{f}_i + \mathbf{f}_j - \left| \mathbf{v}^{ij} \right| \left(\mathbf{v}_i - \mathbf{v}_j \right) \quad , \quad \mathbf{v}^{ij} = \frac{1}{2} S_k^{ij} \left(\mathbf{v}_i^k + \mathbf{v}_j^k \right)$$

• Higher Order Scheme via Limiting (e.g. MUSCL)

Spatial Discretization: Divergence (1)

• Galerkin:

$$\mathbf{r}^{\mathbf{i}} = D^{ij}\mathbf{F}_{\mathbf{i}\mathbf{j}} = D^{ij}(\mathbf{f}_i + \mathbf{f}_j)$$

$$\mathbf{f}_i = S_k^{ij} \mathbf{v}_i^k$$

- Need Consistent Numerical Fluxes (LBB Condition)
 - Different Functional Spaces for *v*,*p* (e.g. Mini-Element)
 - Artificial Viscosity/Stabilization
 - Edge-Based Consistent Numerical Flux

Spatial Discretization: Divergence (2)

Consistent Numerical Flux

$$\mathbf{F}_{ij} = \mathbf{f}_i + \mathbf{f}_j - \left| \lambda^{ij} \right| \left(p_i - p_j \right) \quad , \quad \lambda^{ij} = \frac{\Delta t^{ij}}{l^{ij}}$$

• Higher-Order (4th Order Damping) $F_{ij} = f_i + f_j - |\lambda^{ij}| \left(p_i - p_j + \frac{\mathbf{l}^{ij}}{2} \cdot (\nabla p_i + \nabla p_j) \right)$

Walls: Boundary Conditions

• Walls: Bouncing, Sticking, Gliding, ...

