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

Small droplets travel as a cloud through the air.

Large droplets travel ballistically through the air.
Virus Transmission: Breathing
Virus Transmission: HVAC/Wakes

0.2-0.3 m/s

1 m/s

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Virus Transmission

• Entering the Body: Nose, Mouth, Eyes
• Exiting the Body: Nose, Mouth
  – Sneezing, Coughing, Shouting, Singing, Speaking, ...

• ➔ Transmission Modes:
  – Person-to-Person : Large/Small Droplets
  – Person-Air-Person : Small Droplets
  – Person-Surface-Person : Large Droplets
Droplet Distribution When Coughing

## Sink Velocities of Droplets in Air

<table>
<thead>
<tr>
<th>Diameter [mm]</th>
<th>Sink Velocity [m/sec]</th>
<th>Reynolds-Nr.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0e+00</td>
<td>3.01e+01</td>
<td>1.99e+03</td>
</tr>
<tr>
<td>1.0e-01</td>
<td>3.01e-01</td>
<td>1.99e+00</td>
</tr>
<tr>
<td>1.0e-02</td>
<td>3.01e-03</td>
<td>1.99e-03</td>
</tr>
<tr>
<td>1.0e-03</td>
<td>3.01e-05</td>
<td>1.99e-06</td>
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<tr>
<td>1.0e-04</td>
<td>3.01e-07</td>
<td>1.99e-09</td>
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</tbody>
</table>
Droplet Evaporation

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 (!!)
Viral Load / Infectious Dose

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  – State of Immune Defenses of Victim
  – Timing of Viral Entry (All at Once, Piece by Piece)
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  – Viral Haemorrhagic Fevers 1-10
  – Tuberculosis 1 (!!)

Cov-19: 100-200
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: Prof. A Marm Kilpatrick, University of California-Santa Cruz.
Infectivity of Covid-19

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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: Prof. A Marm Kilpatrick, University of California-Santa Cruz.
Covid-19 vs. Influenza/Flu

• Max Yearly US Deaths From Influenza/Flu: 60K
  – No Lockdowns, No Preventive Measures

  – With Lockdowns, With Preventive Measures
Covid-19 vs. Influenza/Flu

• Max Yearly US Deaths From Influenza/Flu: 60K
  – No Lockdowns, No Preventive Measures

  – 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 → ‘Spitting’
  – Small Droplets → ‘Smoke’
<table>
<thead>
<tr>
<th>Procedure Measure</th>
<th>Large Droplets (spitting)</th>
<th>Small Droplets (cigarette smoke)</th>
<th>Person-Air-Person</th>
<th>Person-Surface-Person</th>
</tr>
</thead>
<tbody>
<tr>
<td>2m/6ft Distance</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
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<tr>
<td>Face Masks</td>
<td>✓</td>
<td></td>
<td>✓</td>
<td>✓</td>
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<td>Periodic Hand Cleaning</td>
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<td>X</td>
<td>✓</td>
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<td>Plexiglass Shields</td>
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<tr>
<td>1-Way Person Traffic</td>
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<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>2x Daily Cleaning</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Nightly UV Cleaning</td>
<td>✓</td>
<td></td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Maximize Fresh Air in HVAC</td>
<td>X</td>
<td>✓</td>
<td>✓</td>
<td>X</td>
</tr>
<tr>
<td>Hard UV Lamps in HVAC Ducts</td>
<td>X</td>
<td>✓</td>
<td>✓</td>
<td>X</td>
</tr>
<tr>
<td>HEPA Filters in HVAC Ducts</td>
<td>X</td>
<td>✓</td>
<td>✓</td>
<td>X</td>
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<tr>
<td>Upper Room UV Cleaning</td>
<td>X</td>
<td>✓</td>
<td>✓</td>
<td>X</td>
</tr>
</tbody>
</table>
Physics
Air: Navier-Stokes, Incompressible

Conservation of Mass, Momentum and Energy:

\[ \nabla \cdot v = 0 \]
\[ \rho v_t + \rho v \cdot \nabla v + \nabla p = \nabla \mu \nabla v + \rho g \beta (T_0 - T) + f \]
\[ \rho c_p T_t + \rho c_p v \cdot \nabla T = \nabla k \nabla T + s \]

\[ \rho : \text{Density} \quad T : \text{Temperature} \]
\[ v : \text{Velocity} \quad c_p : \text{Heat Capacitance} \]
\[ p : \text{Pressure} \quad k : \text{Thermal Conductivity} \]
\[ \mu : \text{Viscosity} \quad \beta : \text{Expansion Coefficient} \]
\[ g : \text{Gravity} \quad f, s : \text{External Forces/Heat Sources} \]
Equations for Diagnostics

- Age of Air
  \[ a_t + \mathbf{v} \cdot \nabla a = 1 \]

- Pathogen Concentration
  \[ c_t + \mathbf{v} \cdot \nabla c = \nabla d_c \nabla c + s_c \]

- UV Irradiation
  \[ I_t + \mathbf{v} \cdot \nabla I = \nabla d_I \nabla I + s_I \]

- ...
Particle Motion and Temperature

• Velocity and Position

\[ \rho_p \frac{\pi d^3}{6} \frac{dv_p}{dt} = D \quad ; \quad \frac{dx_p}{dt} = v_p \]

• Temperature

\[ \rho_p c_{pp} \frac{\pi d^3}{6} \frac{dT_p}{dt} = Q \]
Momentum Transfer

• Drag Force of Each Particle

\[ D_i = \frac{\pi d^2}{4} c_d \frac{1}{2} \rho |v - v_p| (v_i - v_{pi}) \]

• Drag Coefficient and Reynolds-Number

\[ c_d = \max \left( 0.1, \frac{24}{\text{Re}} \left( 1 + 0.15 \text{Re}^{0.687} \right) \right) \quad ; \quad \text{Re} = \frac{\rho |v - v_p| d}{\mu} \]
Heat Transfer

• Heat Flux For Each Particle

\[ Q = \pi d^2 \left[ h(T - T_p) + \alpha \left( T^4 - T_p^4 \right) \right] \]

• Film Coefficient, Nusselt- and Prandtl-Number

\[ h = \frac{k \cdot Nu}{d} \quad ; \quad Nu = 2 + 0.459 \Pr^{0.333} \Re^{0.55} \quad ; \quad \Pr = \frac{c_p k}{\mu} \]
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 \(\rightarrow\) 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: $\Delta$-Scheme (1)

\[
v^{n+1} = v^n + \Delta v^a + \Delta v^p = v^* + \Delta v^p
\]

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

- **Pressure Correction:** $p^n \rightarrow p^{n+1}$
  \[
  \nabla \cdot v^{n+1} = 0
  \]
  \[
  \frac{v^{n+1} - v^*}{\Delta t} + \nabla (p^{n+1} - p^n) = 0
  \]
  \[
  \Rightarrow \nabla^2 (p^{n+1} - p^n) = \frac{\nabla \cdot v^*}{\Delta t}
  \]
Temporal Discretization: $\Delta$-Scheme (2)

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

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

Remarks:
- Residuals of Pressure Correction Vanish for Steady-State
  - Results Not Depend on Projection Scheme
  - Results Not Depend on $\Delta t$
Particle Motion and Temperature

- Position, Velocity and Temperature: ODEs of Type

\[
\frac{du}{dt} = r(x, u_f, u, t)
\]

- Integrated Explicitly; Typically: 4\textsuperscript{th} Order Runge-Kutta

\[
u^{n+i} - u^{n+i-1} = \alpha_i \Delta t \cdot r(x, u_f, u^{n+i-1}, t^{n+i-1})
\]

\[
\alpha_i = \frac{1}{k - i + 1}
\]
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

\[ S_I \sim \frac{1}{r^2} \]

• Shading Possible \(\rightarrow\) Ray-Tracing
  – From Element (Gauss-Points) to UV Lamp
Raytracing With FEM Grids

- Any Point P:
  \[ \mathbf{x}_P = \mathbf{x}_A + \mathbf{x}_{BA} \xi + \mathbf{x}_{CA} \eta + \mathbf{x}_{DA} \zeta = \mathbf{x}_A + \mathbf{G} \xi \]

- \( \xi = \mathbf{G}^{-1} \mathbf{x}_{PA} \)

- Given Input Location, Obtain Output
  \[ \xi_0 = \xi_i + \mathbf{G}^{-1} \Delta \mathbf{x} = \xi_i + \mathbf{G}^{-1} \mathbf{v} \Delta t = \xi_i + \alpha \Delta t \]

- Output Faces: \( \xi_0 = 0 \)

- Get \( \min(\Delta t_i) \), \( \Delta t_i > 0 \) \( \Rightarrow \) Neighbour Element

Ceiling UV In Hospital Room
Coupling of CFD and CCD
Coupling of CFD and CCD

For Each Gridpoint:
- Temperature
- Smoke
- Toxic Substances
- Pathogens
...

3-D to Tria (CCD Background Grid)

CFD: FEFLO

Ellipse/Point to 3-D Body

For Each Pedestrian:
- Position
- Velocity
- Temperature
- Pathogens
...

CCD: PEDFLOW
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
CCD → CFD

As Tet-Mesh

As Spheres
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]:

\[
M \frac{\Delta v_i}{\Delta t} = r_i + f_i \quad \Rightarrow \quad f_i = M \frac{w_i^{n+1} - v_i^n}{\Delta t} - r_i
\]
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:

\[ m \mathbf{v}, t = \mathbf{f} \]

\[ \mathbf{x}, t = \mathbf{v} \]

- m: Mass
- \( \mathbf{v} \): Velocity
- \( \mathbf{x} \): Position
- \( \mathbf{f} \): Sum of All Forces
- Modeling Effort: \( \mathbf{f} \)
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

Madrid Metro Station

• 3/11/2004 Attack
• Did Blast Analysis
• Follow-Up
Madrid Bomb Attack

PEDFLOW

CFD Center, George Mason University
Madrid Bomb Attack

PEDFLOW
Madrid Bomb Attack
Evacuation from Medina Mosque

- Over $10^5$ 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
Examples (2)

• 3 Different Timescales, Depending on Size
  – $O(10^0)$ sec: Fast, Ballistic Drop of Large $d=1.0$ mm Particles
  – $O(10^1)$ sec: Slower Drop of Intermediate $d=0.1$ mm Particles
  – $O(10^2)$ sec: Transport of Small $d<0.01$ mm Particles Through Air

• HVAC Systems:
  – Good Mixers
  – Complex Flowfields
  – ➔ Condusive to Pathogen Transmission
Sneezing in TSA Queues
Sneezing in TSA Queues
Sneezing in Hospital Room

2.25 Mels
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

Sneezing in Subway
Sneezing in Subway

Time: 2.500000
Sneezing in Subway
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

Bathroom Exhaust

Inflow Vents

1

2

3

Door

average_velo Magnitude

0.0

0.1

0.2
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
Hospital Room: Age of Air

- Inflow Vents
- Bathroom Exhaust
- Door
Max Values Measured During 5 Mins

Vent 1

Vent 2

Vent 3

Patient
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: 0
- Points With 4 Cases (Out of 4) Measured: 0

- 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: $\Delta$-Scheme (1)

\[ v^{n+1} = v^n + \Delta v^a + \Delta v^p = v^* + \Delta v^p \]

- **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:** $p^n \to p^{n+1}$

\[ \nabla \cdot v^{n+1} = 0 \]
\[ \frac{v^{n+1} - v^*}{\Delta t} + \nabla (p^{n+1} - p^n) = 0 \]
\[ \Rightarrow \quad \nabla^2 (p^{n+1} - p^n) = \frac{\nabla \cdot v^*}{\Delta t} \]
Temporal Discretization: $\Delta$-Scheme (2)

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

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

Remarks:
- Residuals of Pressure Correction Vanish for Steady-State
  - Results Not Depend on Projection Scheme
  - Results Not Depend on $\Delta t$
Spatial Discretization: Advection (1)

- Galerkin:
  \[ \mathbf{r}^i = D^{ij} \mathbf{F}_{ij} = D^{ij} (\mathbf{f}_i + \mathbf{f}_j) \]

  \[ \mathbf{f}_i = S^{ij} k F^k_i, \quad S^{ij} k = \frac{d^{ij}_k}{D^{ij}}, \quad D^{ij} = \sqrt{d^{ij}_k d^{ij}_k} \]

  \[ d^{ij}_k = \frac{1}{2} \int (N^i_{,k} N^j - N^j_{,k} N^i) \, d\Omega \]

  \[ \mathbf{f}_i = (S^i_{,k} v_k^i) \mathbf{v}_i \]
Spatial Discretization: Advection (2)

• Need Consistent Numerical Fluxes
  – Integration Along Characteristics
  – Taylor-Galerkin/Streamline Diffusion/SUPG/GLS/…
  – Edge-Based Upwinding

• Consistent Numerical Flux

\[ F_{ij} = f_i + f_j - |v^{ij}|(v_i - v_j) \]
\[ v^{ij} = \frac{1}{2} S^{ij}_k (v^k_i + v^k_j) \]

• Higher Order Scheme via Limiting (e.g. MUSCL)
Spatial Discretization: Divergence (1)

- Galerkin:
  \[ r^i = D^{ij} F_{ij} = D^{ij} (f_i + f_j) \]
  \[ f_i = S_{k}^{ij} v_{i}^{k} \]

- Need Consistent Numerical Fluxes (LBB Condition)
  - Different Functional Spaces for \( \mathbf{v}, \rho \) (e.g. Mini-Element)
  - Artificial Viscosity/Stabilization
  - Edge-Based Consistent Numerical Flux
Spatial Discretization: Divergence (2)

- Consistent Numerical Flux

\[ F_{ij} = f_i + f_j - |\lambda^{ij}|(p_i - p_j) \quad , \quad \lambda^{ij} = \frac{\Delta t^{ij}}{l^{ij}} \]

- Higher-Order (4\textsuperscript{th} Order Damping)

\[ F_{ij} = f_i + f_j - |\lambda^{ij}| \left( p_i - p_j + \frac{l^{ij}}{2} \cdot (\nabla p_i + \nabla p_j) \right) \]
Walls: Boundary Conditions

- Walls: Bouncing, Sticking, Gliding, …

- Embedded Surfaces