Molecular Dynamics Like Numerical Approach for Studying Infection Propagation

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Introduction

Molecular dynamics is an N-body method wherein dynamic evolution of interacting atoms and molecules is computationally simulated. It is a popular computational method for studying the mechanical and thermal behavior of nanomaterials and nanocomposites. Social force models [1] of pedestrian evolution utilize the same numerical framework for evolving the trajectories of moving pedestrians. In this paper, we propose an integrated model that merges a social force based pedestrian dynamics theory with a stochastic infection transmission framework to evaluate the propagation of Ebola infection aboard an airplane.

Air travel has been identified as a leading factor in the spread of many different viruses [2]. Pedestrian motion through airports and airplanes leads to susceptible passengers coming into contact with infected passengers and contagion with harmful consequences. The objective of this study is to evaluate the effects of pedestrian movement during air-travel on the spread of infectious diseases. *We do so borrowing numerical methods like molecular dynamics and Monte Carlo analysis from the field of computational materials science.*

Pedestrian Particle Dynamics

We model the motion of pedestrians using a molecular dynamics based social force model [3]. Assuming a pedestrian as a particle in motion, the point mass is subjected to competing forces of a person's desire to travel to a destination while impeded by obstructions (e.g. walls, chairs and other pedestrians) $\overline{f_l^{int}}$ and $\overline{f_l^{ped}}$ respectively. The net resultant force ($\overline{F_l}=\sum \overline{f_l}$) applied on an individual pedestrian is expressed by:

$$\overline{F_l}=\sum \overline{f_l} = \overline{f_l^{int}} + \overline{f_l^{ped}} = m_i \overline{a_l} \qquad (1)$$

The intention force is a function of the desired velocity ($\bar{v}_{0i}$) of pedestrian i heading towards his destination and the actual speed v_i , and is expressed by:

$$\overline{f_l^{int}} = \frac{m_i}{\tau} [\ \overline{v_{0l}}(t) - \overline{v_l}(t)\ ] \qquad (2)$$

Note that τ is a time step and in order to mimic the adjustment of the pedestrian-particle's perpetual motion when approaching other particles in stagnation, we introduce the location dependence on the desired velocity as:

$$\overline{v_{0l}}(t).\overrightarrow{e_1} = (v_A + \gamma_i\ v_B)\ (1 - \frac{\delta}{r_l\overrightarrow{e_1} - r_k\overrightarrow{e_1}}) \qquad (3)$$

where $(v_A + \gamma_i\ v_B)$ represents the desired speed for a single pedestrian in the crowd. Here, γ_i is a random number and δ is the critical distance between two pedestrians in a line at which the rear pedestrian stops moving. The repulsive force ($\overline{f_l^{ped}}$), essential to ensure impenetrability of particles. For this purpose we use the repulsive term of Lennard-Jones potential given by:

$$\overline{f_l^{ped}} = \sum \overline{f_{lJ}} = \sum_{i\neq j} \nabla\varphi(\overline{r_{lJ}}) = \sum_{i\neq j} \nabla[\epsilon \left(\frac{\sigma}{r_{ij}}\right)^{12}] \qquad (4)$$

There are several parameters in equations (1)-(4), some of which like average pedestrian speeds are available in the literature [e.g. 4]. For estimating other parameters, we perform a massive parameter sweep of feasible ranges of parameters using parallel algorithms on supercomputing clusters and correlate it with available experimental data to identify validated parameters (See Figure 1). Figure 2 shows the validated pedestrian movement results which effectively predict the deplaning times and characteristics for multiple airplanes.

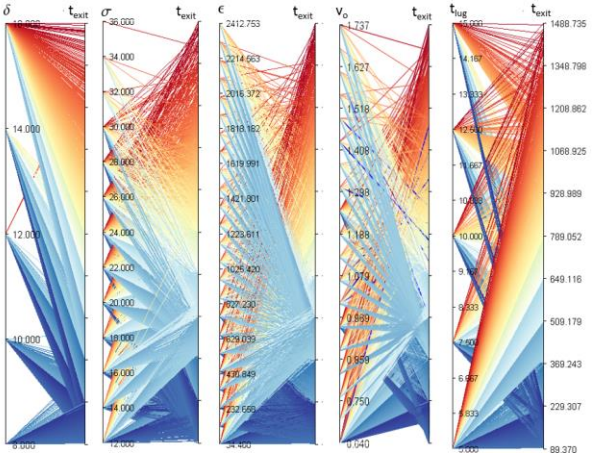

Figure 1. Parallel coordinate plots show the variation of model parameters resulting in different exit times and trajectories.

Infection Dynamics

The pedestrian trajectory information from the above model is integrated with a discrete-time stochastic Susceptible-Infected (SI) model.

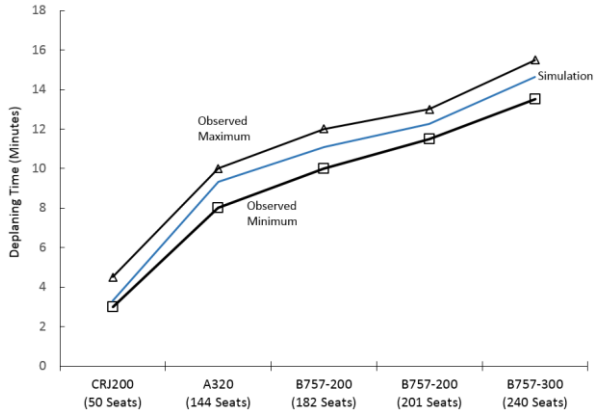

Figure 2. Model results vs. observed deplaning times [5,6].

When the i_c^0 infectives come into contact with m susceptibles estimated by the pedestrian movement model, the newly infected at time t and the probability of their infection can be estimated as Poisson approximation of binomial distribution given by:

$$I(t) \sim Poisson\left(\sum_{c=1}^{d}\left(p_c \sum_{i=1}^{i_c^0}\left(\frac{m_i(t-1)s_{r_i}(t-1)}{N}\right)\right)\right) \quad (4)$$

The probability-distribution of infection transmission (*Pc*) varies depending on the incubation periods and transmission rates for specific diseases and can be estimated by the data available in the literature. Use of Poisson distribution accounts for demographic stochasticity. We used this approach to study the impact of different procedures for boarding, disembarkation, and seat assignment on the number of contacts and consequent spread of Ebola infection for passengers on an airplane.

For example, Figure 3 shows that on a 182 passenger Boeing 757 airplanes, different boarding policies can lead to changes in infection transmission. We have also obtained similar results showing the potential for changes in in-plane movement, deplaning procedure, seating arrangement, and plane sizes in reducing the likelihood of infection transmission. For example figure 4 shows the impact of airplane size on Ebola infection spread. We find that smaller airplanes like 50 seater CRJ 200 are more effective in mitigating infection spread.

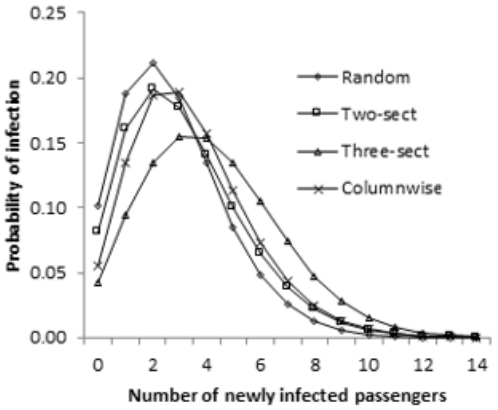

Figure 3. Infection profile with different boarding strategies for Boeing 757-200.

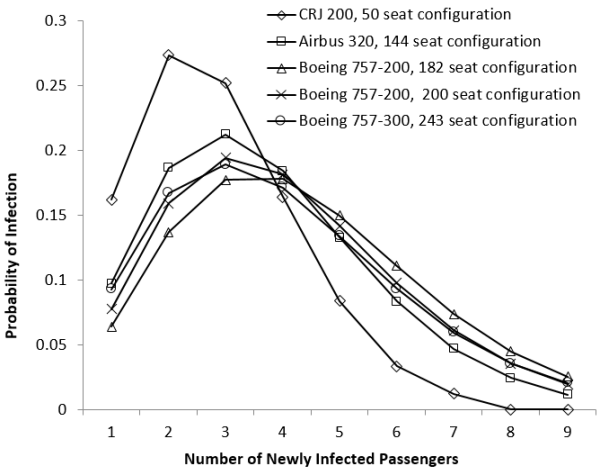

Figure 4. Infection distribution profile for random boarding strategy varying the airplane size.

The approach is applicable for any directly transmitted disease and movement of people in any high density area, for example airport gates, security lines etc. *In the final presentation, we will focus on the parallels between materials modeling methods and this approach for studying infection dynamics.*

References

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