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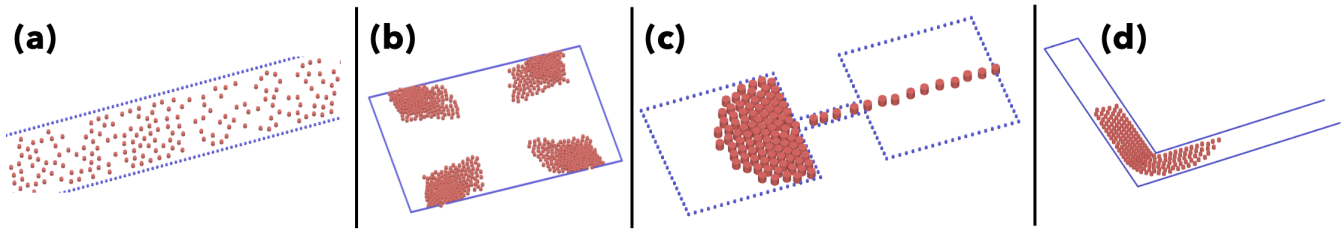

Figure 1: Four pedestrian flow systems, simulated and visualized using computing tools traditionally used for molecular simulation: (a) Unidirectional corridor flow; (b) evacuation of a room through multiple exits; (c) flow through a bottleneck; (d) flow around a corner.

ABSTRACT

Efficient and accurate simulations of pedestrian dynamics are critical for the smart cities of the future. In this work, we present a computational toolbox that accelerates such simulations relative to a popularly used pedestrian simulation tool by leveraging computational frameworks initially developed for molecular simulation. We make the argument that the field of pedestrian dynamics could benefit to a significant extent from a serendipitous interdisciplinary synergy with the molecular-simulation community. We provide arguments and representative examples in support of this premise, demonstrating that molecular simulation tools can be repurposed to solve precisely the same governing equations as traditional pedestrian-dynamics simulation tools, yielding the same results in significantly reduced computational time. We also describe a computational tool that we have developed that streamlines the conversion of indoor maps into boundary conditions for pedestrian simulations.

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CCS CONCEPTS

• **Applied computing** → **Physical sciences and engineering**; • **Computing methodologies** → **Molecular simulation**; **Simulation tools**.

KEYWORDS

pedestrian dynamics, particle-based simulation, high-throughput simulation, automatic geometry generation

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1 INTRODUCTION

Efficient, equitable, and robust prediction and engineering of crowd dynamics is critical for a host of challenges that cities face every day, including managing large-scale flows of crowds, mass transit systems, and emergency response. Quickly and accurately modeling patterns of flow within dense pedestrian environments will be an increasingly important ability for the smart cities of the future. High-performance computational science plays (and will continue to play) an important role in meeting these challenges.

At their mathematical core, all agent-based models for pedestrian dynamics execute a specified set of rules to obtain the trajectory of

each pedestrian [10]. A major class of these models makes use of the concept of "social forces": Pedestrians are treated as particles whose dynamics are governed by inter-particle interactions coupled with goals specific to each individual, all of which can be cast as a (large) system of (coupled, highly non-linear) ordinary differential equations. Since their introduction [6], social-force-based models (SFMs) have a rich history modeling a wide variety of pedestrian dynamics scenarios (as reviewed in [10]), including under emergency circumstances (e.g., [5]) and within complex geometries (e.g., [13]). SFMs have been extensively validated against real-world observations (see, e.g., [16]). Recent extensions to the SFM concept allow for easy assimilation of experimental measurements, which can further improve an SFM's agreement with real-world observations, leveraging developments in data-driven engineering (e.g., [14]) and automatic differentiation (e.g., [12]).

By a stroke of serendipity (or, at least, by the universality of classical mechanics), this task is also the core goal of molecular-dynamics (MD) simulations, which compute trajectories of atoms by tracking the forces acting on each atom over time. To be clear, the fundamental origins of these forces differ in the two cases: At large separation distances, pedestrians are primarily governed by the forces of psychology and atoms by electromagnetism; at short separation distances, pedestrians by elasticity and atoms by quantum mechanics. Nevertheless, because SFM-based pedestrian-dynamics simulations and molecular-dynamics simulations share an identical mathematical framework, it is possible to solve for pedestrian trajectories within the SFM framework using a numerical solver designed for molecular simulation; in other words, one can use "pico-scale science" to produce "pedestrian-scale solutions." It is worth emphasizing that in doing so, one solves *precisely the same governing mathematical equations*, and so obtains the same results.

Our goals in this work are two-fold: First, we highlight why it is not only possible, but in fact highly desirable, to adapt molecular simulation methods for pedestrian dynamics; second, we describe efforts that we have undertaken in order to facilitate this interdisciplinary approach.

2 BRIEF BACKGROUND ON PEDESTRIAN-DYNAMICS SIMULATIONS

SFM-type pedestrian-dynamics simulations and molecular-dynamics simulations both solve for the trajectories of their respective particles by numerically integrating Newton's Second Law, $m\frac{d^2\vec{r}}{dt^2} = \vec{F}$, to obtain $\vec{r}(t)$ for each particle.

In this section, we provide a brief overview of the basic SFM approach for obtaining $\vec{F}$; we refer interested readers to [10] for more detail. Within this framework, the force on each pedestrian is

$$\vec{F} = m\frac{\vec{v}_{\text{des}} - \vec{v}_{\text{inst}}}{\tau} - \vec{\nabla}U + \vec{F}_{\text{near}} + \vec{R}, \tag{1}$$

where the first term constitutes a force (of proportional control) that reduces deviations between each pedestrian's desired velocity $\vec{v}_{\text{des}}$ and their instantaneous velocity $\vec{v}_{\text{inst}}$, mediated over a characteristic relaxation timescale τ (m is pedestrian mass); the second term features an inter-pedestrian energy U, which accounts for each pedestrian's desired amount of personal space; the third term $\vec{F}_{\text{near}}$ represents near-field interactions between physically contacting pedestrians; and the fourth term $\vec{R}$ represents (zero-mean and delta-correlated) noise, which helps break the symmetry of pedestrian-on-pedestrian deadlocks. The exact functional forms of each term, associated length- and force-scales, and magnitude of the auto-correlation of $\vec{R}$ are distinguishing features between different SFMs.

3 METHOD DESCRIPTION AND VALIDATION

We implement the SFM as a two-dimensional (2D) simulation within the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [18], a software package originally developed for molecular simulation in two or three spatial dimensions. It is worth noting that the SFM interaction given in Eq. (1) is not a standard inter-particle interaction implemented in molecular simulation tools; the implementation of this interaction in LAMMPS is one of the important contributions of this work. Following a typical choice made in SFMs [10], we implement an inter-pedestrian interaction energy U that decays exponentially with inter-pedestrian separation distance, with an attenuation lengthscale d_0; this interaction is identical to the (van-der-Waals-free) Buckingham potential [3] used in molecular simulation. In particular, the inter-pedestrian energy for pedestrian i is given by

$$U^{(i)}(r_{ij}) = \sum_{j\neq i} Ke^{-\frac{r_{ij}}{d_0}} \tag{2}$$

where r_{ij} is the separation distance between pedestrians i and j and K is an energy-scale.

We compare our approach against an existing and highly validated SFM implementation, JuPedSim [4, 8], for two-pedestrian interactions. As a first test, we find agreement within 10^{-4} for both U and $|\vec{\nabla}U|$ over a range of separations that capture normal day-to-day pedestrian interactions ($0.1d_0 \leq r_{ij} \leq 5d_0$); both U and $|\vec{\nabla}U|$ are normalized by their values when $r_{ij} = d_0$. As further validation, we compare the results between PSS4PSS and JuPedSim for four canonical systems described in the RiMEA standard [15], a suite of validation scenarios for pedestrian-dynamics simulations (Figure 1). Both PSS4PSS and JuPedSim agree within 10% on the observables of interest in all four test cases. Examples showing the use of PSS4PSS for pedestrian-dynamics simulations are available at [1].

4 KEY BENEFITS OF ADAPTING MOLECULAR SIMULATION TOOLS

The pedestrian-dynamics research community, both academic and commercial, has already developed a considerable body of simulation tools to solve the coupled equations described above, which naturally motivates the question: Why do we need even more tools? In this section, we highlight several of the major benefits to building a "footbridge" between the worlds of pedestrian dynamics and molecular dynamics:

(1) First (and foremost), MD codes are computationally *fast*. This is perhaps unsurprising, since one of the core goals of the MD community is to use *atomistic* simulations to make measurements that are statistically representative of *macroscale* materials (which contain numbers of atoms that are on the scale of Avogadro's number). Since the genesis of the MD method [2] (which recognized that "the essential limitations

of the method are due to the relatively small number of particles that can be handled"), developers have targeted extreme computational efficiency, yielding such codes as LAMMPS that are capable of simulations with $O(10^{12})$ atoms. These codes are designed to scale well on large-scale parallel computing resources with distributed memory, making use of a number of tricks for efficient spatial decomposition. To benchmark particle-based codes, it is common to report performance in terms of "particle-timesteps per second" (PTPS). As shown in Figure 2, we are able to achieve $O(10^6)$ PTPS on an eight-core Intel i7 machine (with better parallel efficiency observed for larger numbers of pedestrians); in comparison, on the same machine, we are unable to observe performances beyond $O(10^5)$ PTPS using JuPedSim, with many simulations performed being closer to $O(10^4)$ PTPS. It is worth emphasizing at this point that the goal of adapting MD codes is *not* to pursue trillion-pedestrian simulations. Instead, the (at least) ∼ 1 order of magnitude speedup described above can be leveraged to perform unprecedentedly *high-throughput* simulations of pedestrians. Such heroic collections of simulations open the door to several previously inaccessible outcomes, including *modeling and optimization in high-dimensional spaces* (critical if a pedestrian flow is being actively engineered through external driving forces) and *meticulous quantification of uncertainties* (by enabling the construction of large-ensemble simulations differing, e.g., in initial conditions).

(2) Despite the existence of several well-maintained and open-source codes for pedestrian-dynamics simulation (see, e.g., [8, 9]), a significant portion of the mature codes in this field are closed-source software and impossible to customize. From the perspective of intellectual flexibility, and for the purposes of studying heterogeneous pedestrian types and equity-oriented questions (concerning, e.g., mobility-impaired pedestrians) that may lack commercial interest at present, there is significant value in being able to access the strong open-source culture in molecular simulation. As an ancillary benefit, simulations carried out in the molecular-simulation ecosystem can also readily take advantage of molecular-scale post-processing and visualization tools (e.g., [17]).

5 EXAMPLES OF PROBLEMS RENDERED TRACTABLE BY THIS APPROACH

In this section, we present pedestrian dynamics problems that our team has studied using adapted molecular simulation code (Fig. 1). For the sake of brevity, our goal here is not to discuss the results of each study; instead, we focus on the core computational challenge of each study that has been rendered tractable (or at least greatly simplified) by PSS4PSS:

- We have used this approach to quantify the effects of social distancing on dynamics in pedestrian counterflows [11]. This study consisted of ∼ 500K simulations, including 512 statistically independent simulations per point in our parameter space in order to compute confidence intervals on transport properties. These simulations, carried out on a large-scale computing cluster, would not have been feasible if the per-simulation cost was even one order of magnitude higher or if the code used could not be readily parallelized.
- We have used this approach to study the effects of obstacles (both stationary and mobile) on pedestrian flows. These simulations benefit from the wide range of existing methods in molecular simulation codes for performing control on target particles, which were initially developed for the purpose of materials characterization (e.g. nano-indentation and microrheology). Due to the rich parameter space of such control schemes, these simulations also benefit significantly from the computational efficiency advantages discussed above.

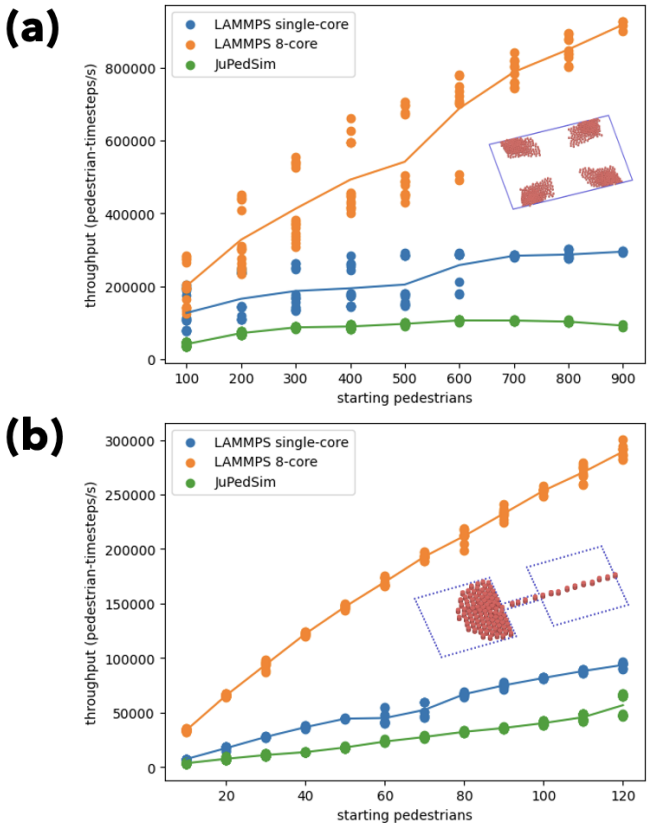

Figure 2: Comparison of computational throughput measured in PTPS as a function of number of pedestrians for PSS4PSS and JuPedSim [8], for (a) evacuation of a room through multiple exits and (b) flow through a bottleneck. For each number of pedestrians, 10 LAMMPS data points are shown (reflecting 10 initial pedestrian configurations); averages are shown as solid lines.

6 A DIGITAL PIPELINE FOR OBTAINING FLOW BOUNDARY CONDITIONS

The problems described above make use of simple confining geometries, e.g., a hallway of constant width. There are numerous tools for developing such simple (and, of course, much more complex)

boundary conditions in molecular simulations (see, e.g., [7]). However, in order to perform simulations in physical domains that are representative of the spatial complexity of real urban environments, it is necessary to have the capability of incorporating geometries with significantly more detail. To this end, previous efforts (see, e.g., [19]) have tackled the problem of automatically converting floor layouts into simulation boundary conditions. In the spirit of bringing this capability to pedestrian-dynamics researchers interested in using molecular simulation tools, PSS4PSS features a novel computational tool (Fig. 2) that is capable of converting indoor maps into geometry input files that are standard in the molecular-simulation community and are compatible with any popularly used MD code.

In this effort, there remain several avenues of important future work, most notably automatic classification of (and subsequent geometry generation for) points of ingress and egress, both at the full-map level and at the individual-room level. Nevertheless, what we have developed so far serves as proof-of-principle that it is possible to generate geometry files that can serve as flow boundary conditions in molecular-simulation environments, and do so in an automated fashion.

7 CONCLUSION

We make the case that the pedestrian-dynamics community could benefit in numerous ways from the adoption of tools used by molecular-scale engineers. Chief among the benefits that we have identified are increased computational efficiency (enabling optimization in high-dimensional spaces as well as uncertainty quantification) and easier access to a broad suite of open-source simulation and visualization tools. It is worth emphasizing that a properly adapted molecular simulation software package will solve *precisely* the same equations that are solved by an existing SFM-based pedestrian simulator; as such, the core difference is in computational efficiency. To foster future work in this interdisciplinary pursuit, we have developed the computational toolbox PSS4PSS, which features an implementation of social-force models in a molecular simulation environment and a workflow that automates the conversion of indoor maps to the boundary conditions used in molecular simulations.

We note in closing that, as with all interdisciplinary work, the flow of information need not be a "one-way street," as evidenced by the following anecdote: Owing to the significant amount of 2D trajectory processing required for this work, our team reported a previously undiscovered error in the popular molecular visualization software OVITO [17] (which was subsequently corrected in OVITO v3.5.3). In other words, the study of pedestrian dynamics can also improve the state-of-the-art in molecular simulation.

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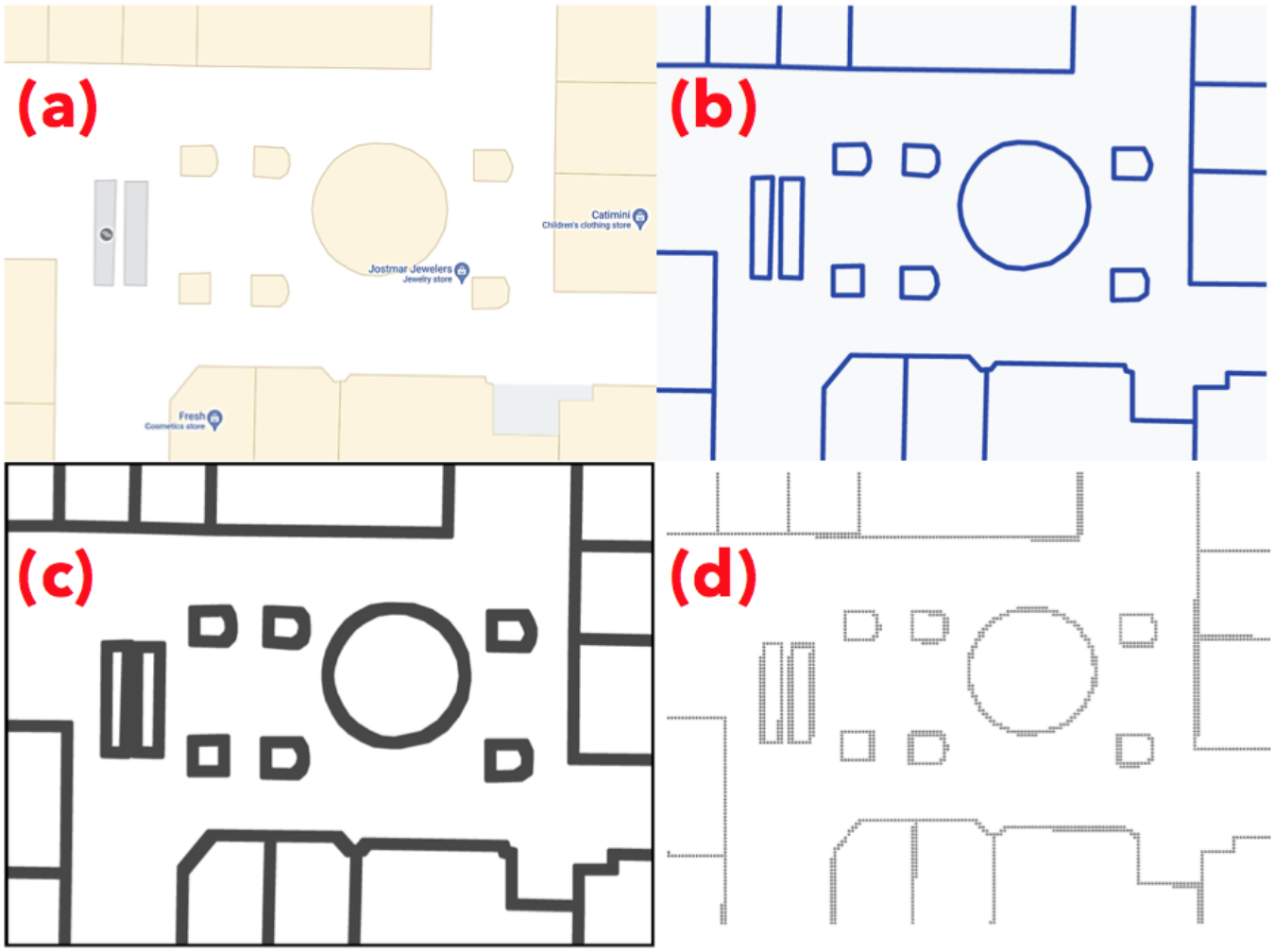

Figure 3: Four stages of the PSS4PSS pipeline for converting indoor maps to geometry files for use in molecular-simulation software: (a) Image of portion of South Coast Plaza (a mall in Costa Mesa, CA), from Google Maps; (b) Labels are removed and edges of significance are detected; (c) Edges are thickened, in preparation for raster scan to identify coordinates of particles that will constitute boundaries; (d) Final geometry file, visualized using OVITO [17] and in a format compatible with LAMMPS [18].