Validation of Molecular Dynamics-Based Structural Damage Models

Research Brief, Volume 2, 2019

PROBLEM

Windstorms currently generate $28 billion in average annual damage and this figure is projected to potentially rise to $38 billion by 2075. Traditional engineering approaches that analyze the resilience of structures *fail to account for non-structural damage* because of the difficulties in modeling such damage. Additionally, even detailed frameworks, like FEMA's HAZUS-MH, provide results only for *categories of building types*. While it is possible to model the sudden impact of loads from hazards like windstorms using such existing frameworks, a methodology does not exist by which to *readily and quantitatively model such damage to unique building designs.*

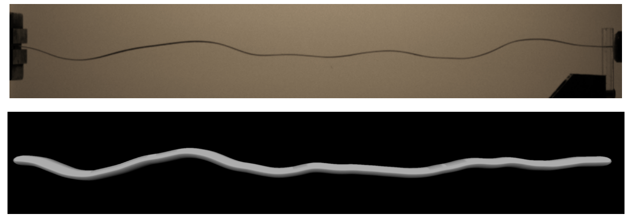


Fig. 1: Typical buckled image for wooden beam. Experiment (top) and simulation (bottom).

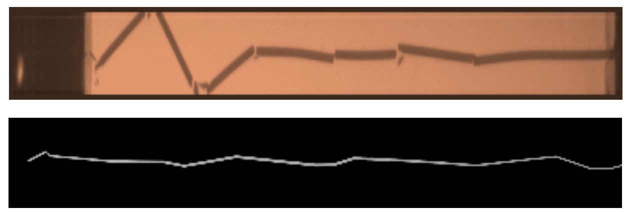


Fig. 2: Typical fractured image shape for pasta beam. Experiment (top) and simulation (bottom).

APPROACH

Inspired by molecular dynamics, we analyze a building not as an ensemble of elements (beams, plates, walls), but as an ensemble of atoms that *interact via forces and moments*, like bonds in molecules. We then apply this coarse-grain model to predict a wide range of effects like *vibrations* (*dynamics*), *fracture*, and *buckling* that can occur under sudden hazard induced loads. To validate this, we focused on smaller elements like columns and beams for which we could easily obtain experimental data in the public literature.

In the experimental setups from the literature, beams of different materials were "shot" by a projectile on one end, and the beam vibrations and fracture (in case of a brittle material) were recorded in video. We chose a wooden beam to demonstrate the elastic response (**Fig. 1**), and a pasta beam (**Fig. 2)** to demonstrate the brittle behavior of our model.

FINDINGS

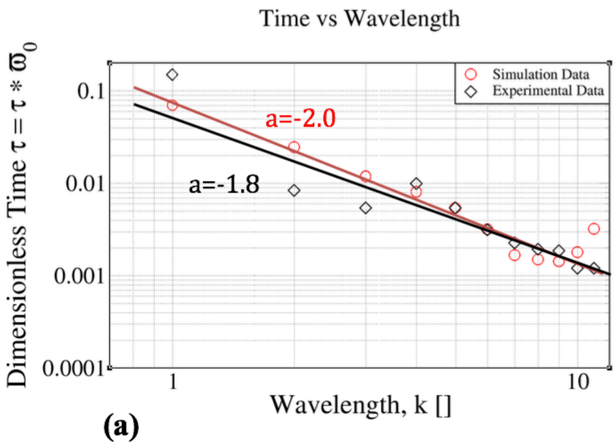
In these types of dynamic instability problems, we observed two conflicting behaviors and validated our results against experimental data*. The first behavior is related to the *dynamics* (vibrations) of the beam, and purely depends on elasticity: the beam shape shifts from higher (or "denser") shapes, to lower (or "coarser") shapes as time progresses (**Fig. 3**). This is called *mode coarsening*. The latter behavior is related to *fracture*, which interrupts this transition from denser to coarser shapes (**Fig. 2**).

*Gladden J.R. et. al. (2005).

WHY DOES THIS RESEARCH MATTER?

- Our approach is more elegant and time efficient than the traditional Finite Element method of structural modeling.
- This is the first coarse-grain simulation of phenomena that are present under real-world conditions, such as *dynamics, buckling* and *fracture*.
- We can now apply an understanding of these kinds of actions in structural elements to entire structures. Fragility curves thus obtained can evaluate the probability of the failure of structures. These probabilities have become key to evaluate the resilience of structures and communities.

This research was carried out by the CSHub@MIT with sponsorship provided by the Portland Cement Association and the Ready Mixed Concrete Research & Education Foundation. CSHub@MIT is solely responsible for content. Authors: Konstantinos Keremidis, Mohammad Javad Abdolhosseini Qomi, Roland J.-M Pellenq, Franz-Joseph Ulm.



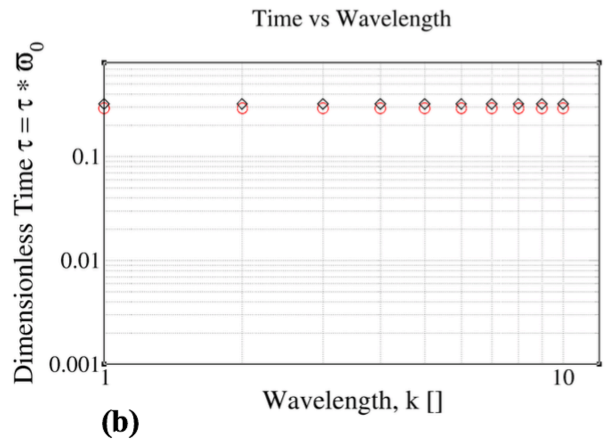


Fig. 3a shows the mode coarsening of the wooden beam. Both simulations (red color) and experiments (black color) predict similar behavior as shown by the linear fit, thus validating our model.

Fig. 3b shows a similar figure for the pasta beam. The beam is brittle; thus, we don't observe a coarsening behavior as in the wooden beam case. Both simulation (red) and experiment (black) show similar pattern.

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