Molecular Dynamics-based Resilience Assessment of Structures

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Bypassing Limitations

Infrastructure damage caused by natural hazards in the U.S. exceeds $50 billion annually, with losses from earthquakes, hurricanes, and fire averaging around $6 billion, $28 billion, and $15 billion, respectively. And, moreover, these costs are trending upward. Such worsening losses, in both their social and economic dimensions, have shifted modern engineering attention towards resilience, which is the ability of infrastructure to recover to a similar or higher functionality level after hazard-induced damage. Yet, despite the growing demand to predict and mitigate such damage, current damage modeling approaches suffer from several limitations, chief among them, level of design detail and speed of calculations.

CSHub researchers have validated a new, physics-based approach that overcomes existing limitations to address the resilience of any building design and its

Key Takeaways:

- The MD approach has significant advantages over traditional methods such as Finite Elements: the absence of instabilities, ease of inelastic implementations, and speed of calculations.
- Built-in resilience (shear walls) and active resilience (sprinklers) play a big role in building resilience.
- Fragility curves obtained on the system scale using the MD model can be used to evaluate the probability of structural failure. These curves are used to calculate the cost of maintenance/repairs in a Life Cycle Cost Assessment (LCCA).

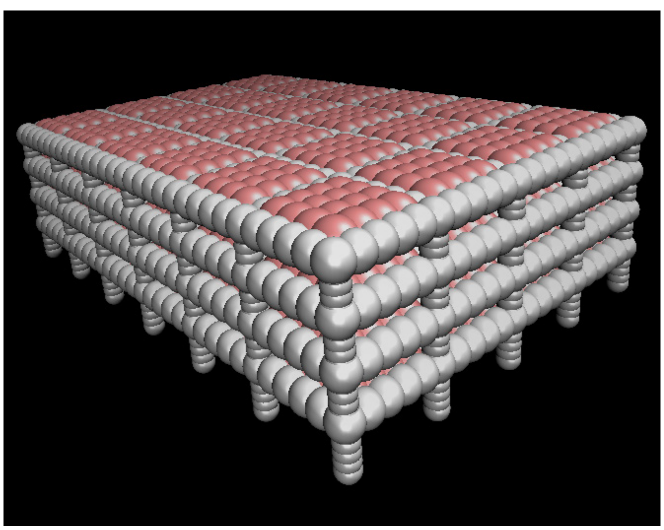

Figure 1: Typical layout of a molecular dynamics model for the case of a DOE Reference Office Building (white masses represent column and beam elements, red masses represent slabs).

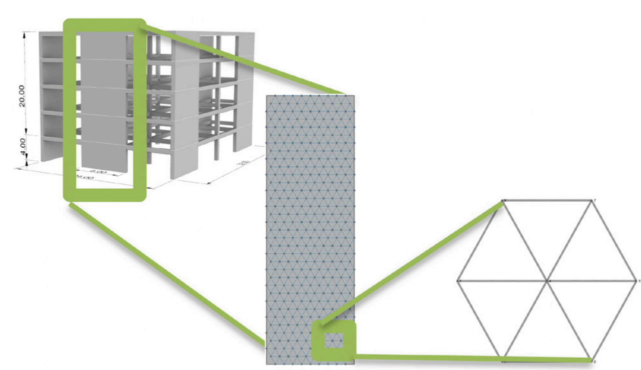

Figure 2. Hexagonal face-centered cubic structure (FCC) pattern used to model shear walls and slabs.

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structural and non-structural elements.

In this brief, researchers expand the building inventory of their model to include shear walls, which are crucial for resisting wind and earthquakes, while also proposing a novel model for sprinklers, which are important for fire resilience. With these enhancements outlined, they use their model to assess the resilience of several building designs to wind, fire, and earthquakes.

The Molecular Dynamics Model

Past work by CSHub has noted that the complexity of buildings is similar to the molecular complexity of materials, in which many strong and weak interacting atoms define the physical properties, ranging from thermal to mechanical. Rather than considering a building as an ensemble of elements (beams, plates, walls), researchers consider a building as an ensemble of discrete mass points ("atoms") that interact via forces and moments, similar to bonds in molecules (**Figure 1**). This approach is called a molecular dynamics model (MD).

In modeling shear walls—and, similarly, slabs—the MD model uses the hexagonal face-centered cubic structure (FCC) as shown in **figure 2**. The advantage of such hexagonal elements is that, since all sides have the same length, they are easier to model and validate. Researchers validated this FCC MD model against conventional finite element models for shear walls and slabs.

For sprinkler modeling, researchers look into the actual behavior of a sprinklered system: the cooling of the room when ambient temperature rises and the structure becomes combustible. While conventional models assume the selection of a specific sprinkler density to manage ambient temperatures, the MD model offers a more quantitative approach: researchers instead model a sprinkler through the physics analogy of thermal "baths," which draws heat out of the system to reduce its temperature—similarly to how a real sprinkler would activate based on ambient temperature to cool the structure.

Sheer Walls and Resilience

Researchers demonstrated the power of their approach by comparing three different design solutions for the case study of an NRMCA proposed building subjected to hurricane, earthquake, and fire: a reinforced concrete design with shear walls (**Fsigure 3a**), a beam-column concrete design (**Figure 3b**) and a wood design with shear walls (**Figure 3c**). In **figures 3d, 3e, and 3f**, they show the designs' damage curves for each hazard: damage curves are a key resilience tool that represent the estimated magnitude of damage for a structure at given load levels.

The damage curves in **figures 3d & e** demonstrate that both wooden and concrete shear walls add substantial resilience in wind and earthquake over a traditional beam-column design, with concrete shear walls having a clear edge. On the other hand, **figure 3f** illustrates how wood deteriorates faster than both concrete designs under fire load while the robustness of a concrete design, especially one with shear walls, instead keeps the building intact.

The fragility curves derived from this MD model can help predict a structure's likelihood of failure and, as a result, inform life cycle cost assessments of repairs and maintenance. Since resilience entails both response and the time to full recovery, quantifying losses through a life cycle perspective is vital. As they advance their model, researchers hope to incorporate non-structural elements as well. Their aim is to publish the results of their work later in 2021.

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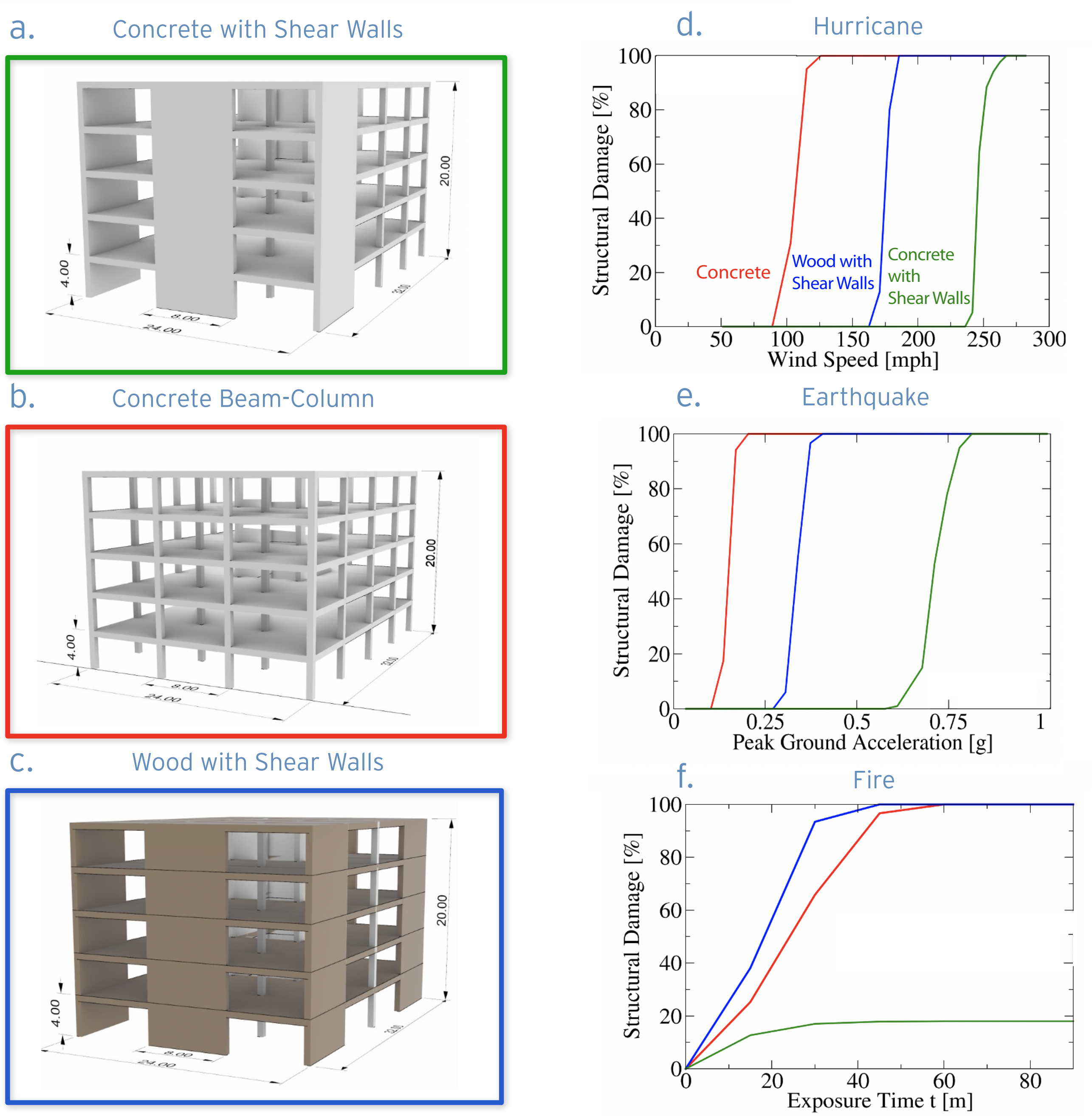

Figure 3: a) Reinforced concrete design with shear walls (in green), b) Reinforced concrete beam-column design (in red), c) Wood design with shear walls (in blue), d) Damage curves for wind, e) Damage curves for earthquake, f) Damage curves for fire.

Related Links:

- CSHub Buildings Research
- CSHub Buildings Resilience Research

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