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# Visualization of Fullerene Fragmentation

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## Abstract

In this paper, we present a novel visualization approach for the analysis of fragmentation of molecules, with a particular focus on fullerenes. Our approach consists of different components at different levels of detail. Whereas one component is geometric but invariant to rotations, two other components are based on the topological structure of the molecules and thus additionally invariant to deformations. By combining these three components, which aim at the analysis of simulation ensembles of such molecules, and complementing them with a space-time representation that enables detailed interactive inspection of individual simulations, we obtain a versatile tool for the analysis of the fragmentation of structured, symmetrical molecules such as fullerenes. We exemplify the utility of our approach using a tightly coupled simulation approach for the dynamics of fullerenes.

**Index Terms:** Computing methodologies—Modeling and simulation—Simulation types and techniques—Scientific visualization; Human-centered computing—Visualization—Visualization application domains—Scientific visualization

## 1 Introduction

Carbon is an integral part of all known lifeforms. Not only is it a vital component in building cells for living organisms, but it also gives rise to a rich variety of potential chemical bindings with exceptional properties. Often, carbon is studied in the form of fullerenes, a category of carbon-based molecules that have seen many uses, including semiconductors and superconductors. Among the fullerenes, $C_{60}$ (Figure 1a), also known as the buckyball, is of particular interest. Having sixty atoms, it is large enough to result in a complex system of coupled atom–atom interactions, and its symmetrical genus-zero structure makes it an ideal example for studying complex carbon bond systems, both experimentally and theoretically. To study bonds of $C_{60}$ experimentally, techniques such as laser pulse excitation are commonly employed, which ionize the molecule and may tear it apart into molecular fragments. While the final products of such decay processes have already been studied extensively, the dynamics of these processes remain an active research topic.

Since the experimental setups are, however, costly and time-consuming, and typically cannot investigate individual molecules, simulation and visualization aid the investigation of laser–fullerene interactions with a special focus on its fragmentation. In this work, we are particularly interested in comparing different simulations among each other, in order to (i) analyze their average behavior, (ii) study the influence of initial parameters, and (iii) highlight interesting phenomena of a fragmentation process. To this end, we introduce novel visualization techniques, encompassing different levels of detail that range from highly coarse (characteristic curves) to extremely detailed (fragmentation trees).

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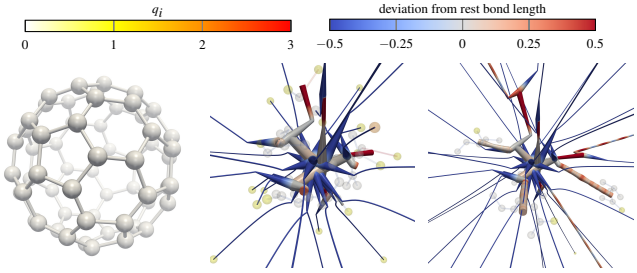


Figure 1: Fragmentation process of a fullerene $C_{60}$ that is positively ionized by 44 elementary charges ($q_{\text{mean}} = 40$, see Section 4). (a) Initial state, not charged, state at (b) $t = 125\,\text{fs}$, and (c) $t = 375\,\text{fs}$ of the fragments. The molecule is represented with the ball-and-stick model together with the fragment tree (colored), our space-time representation of its dynamics. Atoms (balls) are colored by their charge $q_i$ (in elementary charges). The deviation from the bond rest length (in Å) is encoded in bonds (sticks) and in the fragment tree, which is color-coded according to the maximum bond length of the corresponding molecule fragment.

Our simulations are realized in the molecular dynamics framework LAMMPS [11], which is capable of simulating intermolecular forces. Each simulation addresses a single molecule, and follows physical experiments by ionizing individual atoms of the molecule, with Gaussian probability distribution. Ionization happens independently of the position of a given atom, and in turn triggers Coulomb forces that cause charged atoms to repel each other, possibly breaking molecular bonds, and eventually leading to fragmentation.

## 2 Related Work

Molecular dynamics simulations are a common tool for investigating fullerenes [9, 16]. Previous work on the analysis of the resulting data includes an approach based on relative distances, in the context of a low-velocity fullerene fragementation process [4]. This approach shares similarities with our eccentricity-based approach, but considers only two molecules, whereas our focus is on multiple molecules (the molecule fragments).

As for the visualization of chemical processes, Wang et al. [15] present several approaches that, using machine learning techniques, build a hierarchy of the most important reactants (which correspond to the fullerene fragments in our application). Their approach shares similarities with our fragment tree approach but does not explicitly address the time-dependency of the fragmentation process. Regarding the analysis of the fragmentation distributions, they plot molecular size with respect to time, whereas we target the visualization of fragment holes due to the particular structure of fullerenes. Ahlstrom et al. [1] present a generic analysis approach that clusters trajectory snapshots, and employs techniques from network analysis. Their approach does not take into account symmetries that are inherent to fullerene fragmentation, though. More weakly related works include visualization of time-varying graphs, where nodes typically represent distinct objects. In this context, feature-based visualization, for example of communities [13] and group structures [14], is