Visualizing the Energetics of the Dissociation of a Metastable Molecule

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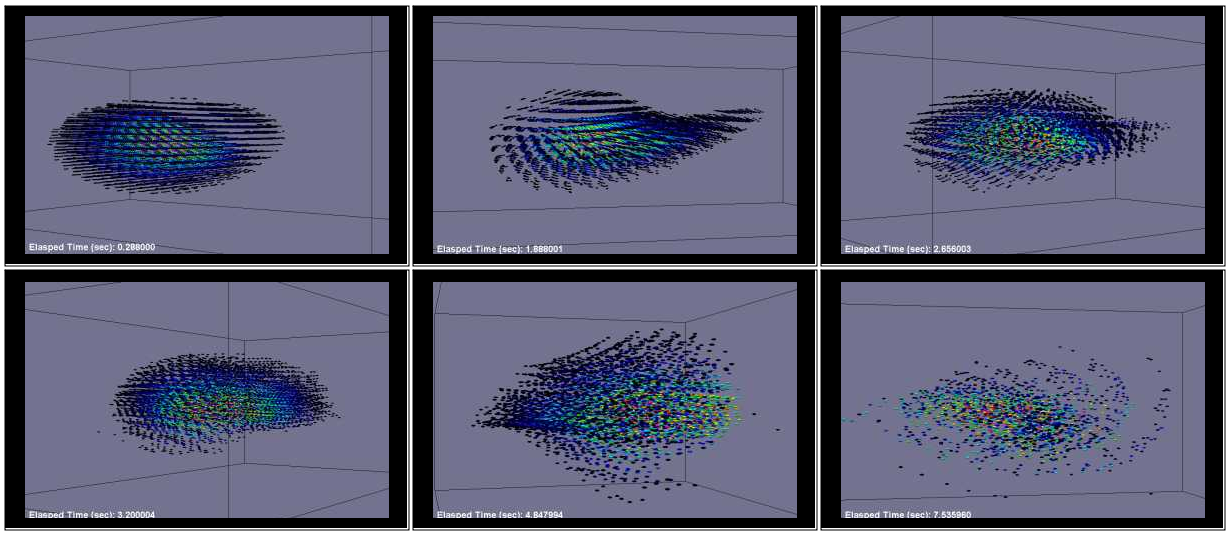

Figure 1: Six time steps from the quantum chemistry animation showing the lifespan of the particles present in the metastable molecule.

Introduction

Shown in Figure 1 is the simulation of the energetics of the dissociation of a metastable molecule. The simulation was computed by Dr. Robert Wyatt, a Professor of Chemistry at The University of Texas at Austin. Dr. Wyatt's simulation uses a model molecule composed of two fragments, A and B. Starting from the molecular state AB, the simulation computes the probability that, under any given conditions, AB will dissociate into the separated components A + B. This may seem like a toy problem, but in real life many molecules demonstrate metastable behavior--a propensity to dissociate--and the work that this simulation is doing may ultimately have an impact on studies of the energetics of larger molecules. An important class of these is biomolecular. This work may be particularly applicable to energy transfer problems in biological systems.

It can certainly have more immediate application for analysis of the many dynamical processes occurring over very short distances and very short times in chemical physics. These include reactive scattering, photodissociation, and reactions seen in the new field of "femtochemistry." This field has been opened by the development of lasers with ultrashort pulses that help scientists trap and record intermediate reaction states with extremely short lifetimes--on the order of femtoseconds (one thousandth of a trillionth of a second).

In 1999, Wyatt and his student Courtney Lopreore (now at the Salk Institute in La Jolla) developed a method they called the quantum trajectory method (QTM), which solves the

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equations of motion to find quantum trajectories for "fluid particles." The solution unfolds in the Lagrangian ("moving-with-the-fluid") reference frame, eliminating the need to solve the problem on a large grid or mesh. The development of this method stimulated many more investigations by dozens of theoretical chemists, and they quickly determined that the approach gives results that are as accurate as similar calculations based on direct solutions to the Schrödinger equation.

Visualizing Quantum Chemistry

The "fluid" shown in the images in Figure 1 is the *probability density* discretized into small "particles." It is the motion of these particles that enables Dr. Wyatt to visualize the outcome: the number of particles escaping from the system at the lower right, for example, represents the overall probability of dissociation at a given energy. The tendency of the molecular system to remain intact is represented by the high-probability-density particles (colored red) that remain in the center of the picture; low-probability-density particles are colored blue.

The goal of the visualization is to interactively display the particle trajectory for simulated probability density with the hope of viewing and determining how the molecule dissociates. Traditional methods for displaying these particles were accomplished using tools such as MatLab and Tec Plot. These tools, however, do not allow all requirements to be met. MatLab does not support interactive display, and Tec Plot does not allow interactive display with multivariate visualization (the display of multiple values of interest per particle). A new system for the interactive display (using OpenGL) of multivariate particles has been developed to exploit new techniques for facilitating fast random access of memory.

File mapping is used to load the simulated data (793 trajectory times with corresponding particle positions and densities) into the virtual address space of the application, allowing for fast random access of the file's contents. The user can interactively view the particles by specifying a time interval. Catmull-Rom splines were used to interpolate between simulated time steps, with the simulated data acting as control points on the spline. Additionally, each particle has an associated life-span that is decremented over time. When the particle has died, meaning that the life-span of the particle is <= 0, the particle is removed from the display.

The particles are shown as spheres to allow for a three-dimensional display. Each sphere is assigned a color based on its density. A particle with a small density value is black and a particle with a large density is white. The life-span of the particles is mapped onto the spheres by mapping translucency. The older a particle is, the more transparent it becomes until it dies and is removed from the display.

The interactive particle visualization that was developed gives a powerful method for gaining additional insights into the behavior and characteristics of particle dynamics in quantum chemistry. Additionally, it serves as a pedagogical tool for interested students in fundamental studies of chemical dynamics. Future work will focus on allowing specific trajectory information to be displayed by incorporating streamers and other particle behavior, and will study the interactive manipulation of very large particle systems.