Virtual Reality Visualization of Parallel Molecular Dynamics Simulation

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Abstract:

When performing communications mapping experiments for massively parallel processors, it is important to be able to visualize the mappings and resulting communications. In a molecular dynamics model, visualization of the atom to atom interaction and the processor mappings provides insight into the effectiveness of the communications algorithms. The basic quantities available for visualization in a model of this type are the number of molecules per unit volume, the mass, and velocity of each molecule. The computational information available for visualization is the atom to atom interaction within each time step, the atom to processor mapping, and the energy rescaling events. We use the CAVE (CAVE Automatic Virtual Environment) to provide interactive, immersive visualization experiences.

1 Introduction

Molecular dynamic simulations are increasingly being used to perform simulations of materials and in the modeling of drug compounds. The validation of these simulations is done by comparing the results of test cases against known results. The numeric results can be visualized to give the user a more intutive feel of what is happening. In addition, the visualization can be used to give feedback on the parallel algorithm. The CAVE is used as a tool to address both of these visualization issues.

The use of the CAVE as tool a to display numerical results in a easy to understand form has proven quite successful [5]. This visualization displays an atom's motion within the area of the simulation along with a selected atom's interaction with its neighbors. Periodicity of the simulation is illustrated through the generation of shadow boxes. Rescaling events, which are performed by the simulation to maintain a constant temperature and pressure, are visualized by a flash of red in the background.

The use of a three dimensional environment such as the CAVE allows for the dynamics of the simulation to be seen in an intuitive inside out fashion. The CAVE environment immediately allows for a simple verification of the correctness of the simulation, along with a visual feedback as to how well the parallel algorithm is working.

2 Molecular Dynamics Simulation

Traditionally molecular simulations involve solving systems of equations dealing with the motion of each atom in relation to every other atom in the system. The motion of each individual atom is the result of a variety of different forces; such as forces due to bonds, Coulomb forces, or van der Waals forces. Coulomb forces are the most computationally intensive due to the interaction of each atom to all other atoms in the system [7].

The primary motivation for this work is to be able to develop an intuitive understanding for interaction

decomposition (force decomposition) parallel molecular dynamics alogrithms that have recently been developed [7, 4]. In these methods interactions are assigned to processors (in some cases as few as one interaction per timestep could be assigned) instead of atoms or regions of space. These interaction methods have the advantage of scaling beyond the historical difficulty of one processor per atom, thus opening up the realm of "fine grain" molecular models which have the possibility of accelerating fixed scale molecular simulations via large-scale parallel computer engines. This work has been motivated largely by the need to solve molecular structure (e.g. folding) problems on teraFLOP class machines that will have on the order of 10,000 processors without the need to scale the molecular simulation to 1,000,000's of atoms.

Because interaction decomposition methods require complex mappings of force matrices to processors, interactive 3D visualization can be used to provide visual evidence of algorithm correctness when testing new methods and can also be used to determine if load balancing strategies are working.

The ideal visualization would include indications of which processors are mapped to which interactions (represented in the visualization as links between atoms) and to show the degrees of clustering (load imbalance) across the range of processors.

Short-range force molecular models can be very accurate and scale linearly. For the purposes of our work, which is to demonstrate the feasibilty of interaction decomposition for future large-scale computers, short-range models are also simple enough to quickly experiment with alternative fine-grain algorithms.

3 Parallel Version of Simulation

The reason for this version of the simulation is to address what is believed to be the future of massively parallel machines (MMP) in the next few decades [1]. This simulation can scale quite easily to a MMP with up to 1,000,000 processors.

4 VR and the CAVE

Virtual reality (VR) is quickly becoming a useful tool in scientific visualization [2]. VR allows for the scientist to be immersed in his/her data and to directly interact with it. VR is defined as surround vision, stereo cues, viewer-centered perspective, real-time interaction, tactile feedback, and directional sound [6].

The CAVE is a virtual reality environment originally developed at the Electronic Visualization Laboratory at the University of Illinois at Chicago, and currently being developed with National Center for Supercomputing Applications (NCSA) and Argonne National Laboratory (ANL)[3]. The CAVE fulfills the VR requirements of surround vision by creating a large field of view by projecting images onto two walls and the floor of a ten foot cube (See Figure 1). Stereo cues are provided by displaying images, sequentially showing the left eye view followed by the right eye view. Then coupled with LCD shutter glasses which are switching the view each eye receives; images can be seen in a three dimensional state. The correct viewer centered perspective is accomplished by constant feedback from an electromagnetic tracking system. The tracking system constantly updates the users location in the CAVE to the CAVE control software, so that the correct view can be calculated.

Interaction of the user with his/her data is accomplished with the wand, a three dimensional equivalent to the traditional workstation mouse. The wand has three buttons that can be programmed to interact with the data in application specific manners. In addition a two-dimensional joystick, that is commonly used for navigation is available.

5 Implementation

In implementing this visualization in the CAVE, we needed to address two issues. The first was the issue of the data to be visualized, and what information was available from that. Secondly, how to actually visualize the data and interact with it.

5.1 Simulation Data

The simulation generates a data stream consisting of event tokens and associated data.

Tokens are generated for:

- (\$) Time step
- (1) Atom position and velocity
- (S) Velocity rescaling
- (F) Neighbor lists

For each time step, a corresponding event token is generated. Between time-step event tokens are a list of every atom in the simulation. For each atom, a three dimensional vector is given for its current position and an additional vector for its velocity. For

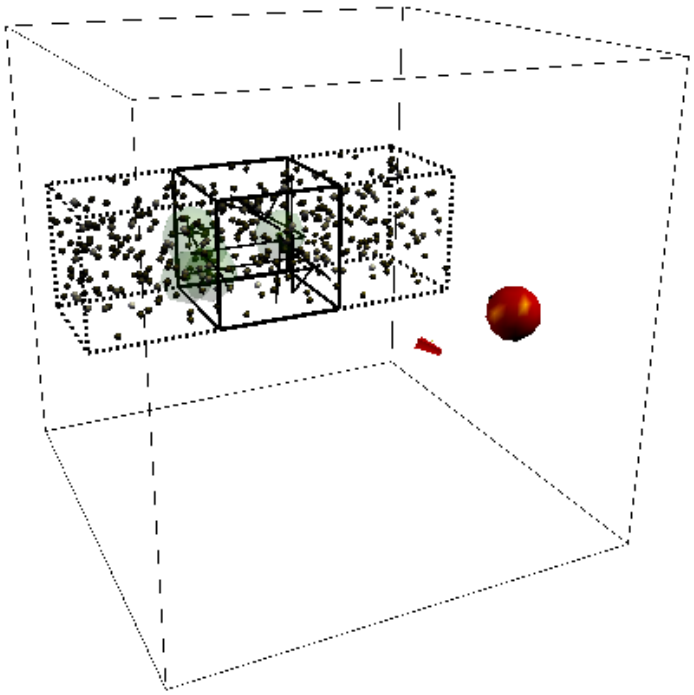

Figure 1: Outside view of the CAVE running visualization of molecular dynamics simulation. The dark sphere and cone represent the user and wand respectively.

selected atoms, there is also a neighbor list which identifies all the atoms the simulation is using in its short range calculations. When a rescaling of the velocities is required, a rescale event is generated.

An excerpt from a typical data file is given below:

```
1 124 .3725E+00 .2211E+00 .2241E+00 -.7435E-04 -.4863E-03 .6604E-04
1 125 .3942E+00 .3273E+00 .2541E+00 -.2381E-04 -.2045E-03 -.3736E-03
F 10 12 14 15 28 33 34 35 39 110 114

S Scale event occurred at this time step
$ New time step
1 1 -.2412E+00 -.1150E+00 -.6166E-01 .4571E-03 .8204E-03 .9739E-03
1 2 .4824E+00 .1737E+00 -.4129E+00 -.3388E-03 -.1228E-02 -.6125E-03
1 3 .4683E+00 -.2930E+00 -.7010E-01 .5872E-03 -.4422E-03 .1118E-03
```

5.2 Visualizing and Interacting with Data

We try to visualize the data in the most intuitive manner possible. The simulation is modeling a real life phenomena and should represent that phenomena in a relatively literal fashion. Since the simulation is modeling the behavior of atoms in an enclosed space, we show the visualization as scaled-up atoms and depict the enclosed space with a simple outlined box. In the examples given, the enclosed space being simulated is 28 angstroms to the side, containing 125 atoms, and we scale it to 3 feet per side. To enhance the visualization, we exaggerate the scale of the atoms, which are represented as spheres. The velocity of each atom is represented by its color with the slowest atoms being shown as blue spheres and the fastest atoms being red spheres. The range of velocities is then interpolated from blue to red over eight steps.

The space in which the atomic movement is being simulated is periodic and we show that feature with shadow boxes on the outside of the main enclosed space. In the shadow boxes, we replicate the position of atoms from the other side of the enclosed space, to show that they are influencing local atoms. (See Figure 2). The entire space is projected three feet up from the floor of the CAVE and is projected into the CAVE three feet from the back wall, allowing the users to step into and around the data.

The sample data set consists of 1000 time steps, but could be any arbitrary number of steps. We animate the time steps at approximately 10 steps per second, giving relatively smooth animation of the atoms in the

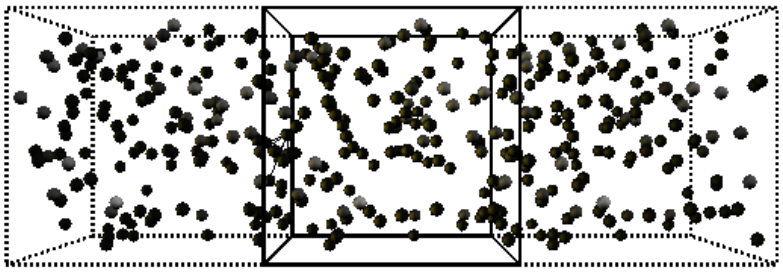

Figure 2: Representation of molecular dynamics simulation in the CAVE.

space. The user can control the animation by using the wand buttons. The left button causes the animation to run backwards, the right causes it to run forward and the middle button pauses the animation. While paused, the left and right buttons single step backwards or forwards through the time steps. When a rescaling event occurs, the normally white background is set to red. When the animation is running, this appears as a red flash in the background.

While it was satisfying to see the movement of the atoms on the whole, that is, as a system, it was difficult to follow the path of a single atom, or to see any history in the system. We decided to add a feature that allowed the user to select an atom, or group of atoms, to be followed and to leave a trail of its prior path (See Figure 3). The user selects an atom to leave trails while the visualization is paused. The left/right axis of the joystick is used to cycle through the atoms, highlighting them one at a time. At the desired atom, the user stops and then rotates the joystick upward to select the particular atom to leave a trail. Selecting it again in the same manner toggles off that feature for the atom.

Another feature we added was to provide the user the ability to select an atom or group of atoms around which to display the radius of interaction being used by the simulation. Using the pause button and joystick as described above, the user rotates the joystick down to toggle the 'show-radius' state of the selected atom. We show the radius as a semi-transparent green sphere around the atom (See Figure 4). This feature is particularly useful when we are viewing the neighbors of an atom. Neighbors are defined as those atoms within the radius of interaction of a given atom. We show those by connecting a line to each neighbor from the subject atom. By turning on the radius sphere, we can verify visually that the simulation is correctly assigning the interactions.

6 Conclusion and Future Plans

We find that by using this visualization, the users can satisfy their intuition on the workings of the simulation and verify the correctness of the interaction assignments.

In the future, we expect to show system energy at each time step, allowing for visual verification of the system rescaling events. We expect to connect the visualization directly to the simulation, allowing the user to control the simulation through manipulation of variables such as number of atoms and system energy level. This direct connection will provide for real time visualization of the output of the simulation.

A future feature we want to add is a display of the processor utilization and the ability to remap interactions to processors on the fly, displaying various performance statistics.

Acknowledgments

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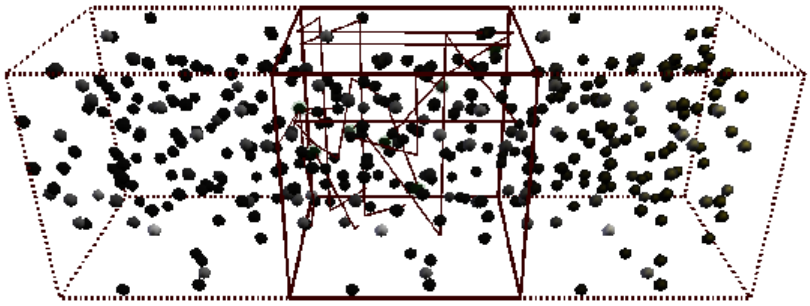

Figure 3: CAVE visualization showing paths of atoms during the molecular dynamics simulation.

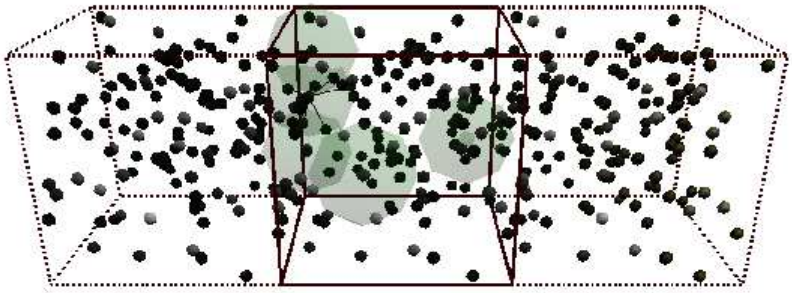

Figure 4: Molecular dyanmics simulation visualized in the CAVE, where the small dark spheres represent atoms and the larger grey spheres represent the radius of interaction.

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