Visualization of Atomistic Simulation Data for Spatio-Temporal Information

Dipesh Bhattarai and Bijaya B. Karki

Department of Computer Science

Louisiana State University

Baton Rouge, LA 70803, USA

ABSTRACT

We have proposed a scheme to support interactive visualization at space-time multiresolution of the atomistic simulation data. In this scheme we have adopted two perspectives that differ in their purposes and in the way they process and render the data. First, the complete or nearly complete dataset is rendered using animation, particle-pathline and color-mapped-dimension techniques to achieve an overall idea of the spatio-temporal behavior of the atomic system under consideration. Second, additional data are generated on the fly and analyzed/visualized using a combined graph-theoretic and statistical approach to gain better and more detailed insight into the desired spatio-temporal information. It is also shown that the proposed approach can greatly assist us to better understand various important atomistic (molecular) properties and processes including bond-breaking/reconstruction, radial distribution, atomic coordination, clustering, structural stability, defects and diffusion.

Keywords

Scientific visualization, Molecular dynamics, Space-time dataset, Cluster analysis

1. INTRODUCTION

Adoption of visualization approach towards better understanding of a given real material system at atomic (molecular) scale has drawn much attention over last several years [Hum96, Kokaji99, Kokaji03, Crysm, Sharma03]. One major challenge is how to extract as much spatio-temporal information as possible from highly accurate data produced by computationally intensive quantum mechanical simulations. The first principles molecular dynamics (FPMD) algorithm based on interatomic interactions derived within the quantum mechanical framework (such as density functional theory) can typically deals with several tens to several hundreds of atoms [Codes]. Typical simulation times are in picoseconds, which translate to a few thousands of FPMD steps. Thus, the simulation data are three-dimensional (discrete degrees of freedom defining the positions of atoms) and time-dependent in the nature.

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In this paper, we propose an effective-efficient scheme of visualization of the atomistic simulation data at space-time multiresolution. To the best of our knowledge, no such systematic approach has previously been proposed although a large number of atomistic (molecular) visualization studies have been reported over the years (see the Related Work Section). Here, we only deal with data sets produced by FPMD simulations, which are generally much smaller than the data sets produced by the classical molecular dynamics (MD) simulations [sharma03] based on empirical or simplified interatomic interaction potential model. However, given the high accuracy of the FPMD data, it is important to extract detailed quantitative and qualitative information hidden in the data. For this purpose, instead of just focusing on direct rendering of the given data, additional data (containing more quantitative information) that usually have to be extracted by some other means are extracted and rendered on the fly. This allows us to gain better insight at multi space-time details of the data (in other words, to extract the global as well local spatio-temporal behavior) for important information such as bonding, pair correlation, coordination, structural units and complex clustering, structural stabilities, defects, diffusion and other dynamic processes.

In the past, the first-principles simulations were mostly performed for crystalline systems in which

the symmetry constrains the simulation size (often unit cells with periodic boundary conditions are used) as well as the atomic configuration (a few free positional parameters need to be considered explicitly). For example, a widely studied material, MgO in its conventional simple cubic structure requires only 8 atoms whose positions are fixed by the cubic symmetry. Now due to the rapid advances in the computational resources/capabilities, the computational studies of defective crystals (such as ones containing vacancies, impurities, dislocations or grain boundaries) and disordered systems such as liquids are increasingly becoming common and precise [Chel01, Karki05, Stix05, Alfe05]. Such parallel simulations often require much larger atomic systems and the crystal symmetry is violated partially or completely. For example, the data for the liquid MgO used in this study were obtained for the atomic system consisting of 216 atoms and a total of 648 positional degrees of freedom need to be explicitly taken into account [Karki05].

The atomic configurations of our interest are represented by the simulation-produced time-varying 3D data. Additional attributes such as charge density, energy, forces, stress- and strain-fields are often associated with these atomistic data. Here, our proposed multi space-time resolution approach deals only with the positional data for constituent atoms as a function of time. This approach is expected to represent a more complete visualization than what currently exist and is also expected to be of an increased importance, particularly in the case of FPMD simulation data sets to extract a variety of structural and dynamical information in both qualitative and quantitative manner. Such knowledge is highly desirable as it forms a basis for understanding different macroscopic properties of materials of substantial scientific and technological importance.

The paper is organized as follows: The Section 2 contains a quick review of previous related work. We present our approach in the Section 3 and explain the proposed visualization model with the details of various rendering algorithms incorporated into it in the Section 4. Important implementation and performance details are presented in the Section 5. Finally, the Section 6 concludes with future directions.

2. RELATED WORK

A lot of work has been done in atomistic (molecular) visualization and analysis for which numerous applications, both commercial and public domain, currently exist. The common examples include VMD [Hum96], Molscipt [Krau91], XcrysDen [Kokaji99, Kokaji03], CrystalMaker [Crysm] and amiraMol [amira]. Both Visual Molecular Dynamics (VMD), which were originally designed for biomolecular systems can now be used for general purpose. XCrysDen can visualize crystalline and molecular structures with ability to superimpose the charge densities on them. Similarly, commercial packages such as CrystalMaker and amiraMol support similar level of interactive 3D visualization, the former being able to handle up to a couple of billions of atoms. Besides, examples of the specific-purpose programs are also abundant [Li05], which include Rasmol, AtomEye, Aviz, Atomsviewer, gOpenMol, VASP DataViewer, PyMD, a few to name. Majority of these applications exploit 3D computer graphics suitable for personal computers and some also support immersive and interactive visualization requiring specialized hardware such as CAVE or Immersadesk system.

In general, the existing visualization systems share many features given below:

- A wide variety of representation (rendering and coloring) modes such as balls, points-and-lines, balls-and-sticks, space-fill and polyhedra
- Real-time manipulations such as rotation, translation, scaling and selection
- Measurement of distances, angles, and dihedrals
- Crystalline properties (e.g., switching between primitive and conventional cell settings, displaying the Wigner-Seitz cell and Brillouin-zone)
- Animations (particularly, for MD simulation trajectories) imported either from files or from a direct connection to a running MD simulation
- Support for a variety of database files from a variety of simulation and experimental sources.

To the best of our knowledge, these visualization systems have a little, if not at all, capability to visualize data at multiple-time and length scales. Several of them are designed to be of general purpose and for that very reason they come short of fulfilling various domain specific requirements. Given a high accuracy of the spatio-temporal atomistic data, our objective here is to extract as much information (both visual and statistical) as possible. For instance, we want to visualize coordination, clustering behavior and diffusion, both at local and global scale and varying with time.

3. VISUALIZATION APPROACH

In a typical molecular dynamics (MD) simulation [Allen87], initially a system is defined by a group of properties that represent atomic types, atomic positions, and constraints that have to be satisfied. Let S be the collection of $\{P, T, C\}$ describing the system, where $P = \{p \in X \subset R^3\}$ (X demarcates the simulation box) is the set of the atomic positions in the system, $T = \{t \in Types\}$ is the set of the atomic types, and C is the set of constraints, which have to

be satisfied by the system. As the simulation progresses, during each intermediate step, a new system configuration is generated, i.e. over each MD step. Collection of S's over the simulation time duration describes the system dynamics, i.e., $D = \{S_i\}$. We approach the atomistic visualization problem in the following three ways.

3.1 Spatial Proximity Analysis

Given a snapshot of the system dynamics, S_i, it is possible to gather information about the spatial proximity of individual atoms to each other, and their collective tendency to form a structure. The structure can range from a regular polyhedral unit to a more complex cluster. In order to fully detect and characterize such structures, one should be able to visualize spatial variations in bond-lengths, bond-angles and coordination environment. It is likely that the bonding and coordination environment for a given atom type is not uniform throughout the system. Radial distribution function, coordination number and compositional disorder are computed and used in subsequent clustering. Also, polyhedral structures may vary in their types and degrees of distortion, and in their arrangements; whether they exist in isolation or form a network. Clusters of different sizes and shapes are computed and visualized.

3.2 Temporal Proximity Analysis

As the simulation progresses, the constituent atoms move in different directions to different extents. A common way of representing the dynamics is animation, which renders the atoms in 3D space as a function of time. Another way is quantification and visualization of the extent of a constituent atom's drift from its initial position or mean position to give further insight into the dynamics of atoms at different times. Temporal clustering for individual atom is then quantified by finding a sphere which is just big enough to enclose all the positions of the atom in 3D space. Center of such a sphere is the centroid of the set of positions an atom occupies during the simulation, and radius is the distance to the farthest position from the center. We also use path-lines - the trajectories of individual atoms in time - to gather information about the dynamics of the individual atoms.

3.3 Spatio-Temporal Analysis

The spatial proximity analysis or temporal proximity analysis alone does not show the complete picture of the system structure and dynamics. It is necessary to integrate together the two types of analyses to visualize how the proximity relationships among the atoms (spatial information) vary over time (temporal information) using animation. For instance, an animated system shows the formation and breakage of bonds and their variation over the time thereby giving overall visual perception of the dynamics. Other properties such as pair correlation, coordination environment, structural units and clustering are also animated. The animation in this way, however, gives an instantaneous view of the dynamics. The MD simulation represents a statistical ensemble. So, it is preferable to visualize the time-averaged and finite-time-span behavior of such an ensemble. For instance, it is interesting to see whether a given structural unit is stable during the whole simulation period. If not, we better know what percentage of time and how many times, the structure is on the scene.

4. VISUALIZATION MODEL

Our visualization model adopts different rendering and analysis techniques [Sch97] and hence it consists of several modules to support the three-types of analyses introduced earlier in the Section 3. The current model represents a major step towards these endeavors. It is worth to mention two important points related to how the model deals with data. First, some modules directly render the given positional data whereas others render the new data, which are extracted from the original data on the fly. Second, some modules render the complete or significant amount of the data at a given instant whereas others render a subset of the data (local in space and time). Thus, our various visualization/analysis modules can broadly be put into two categories, namely, *complete data rendering* and *local/extracted data rendering*. For demonstration purposes, we use the FPMD simulation data for MgO and $MgSiO_3$, which are among the most widely studied materials due to their substantial geophysical significance for the Earth's mantle. Liquid phases and defective systems are analyzed using the 3D positional data for the systems containing 64 and 216 atoms for MgO, and 80 and 160 atoms $MgSiO_3$ [Karki05, Stix05]. Data per simulation have been collected over up to 5000 FPMD steps.

4.1 Complete Data Rendering

Animation

Animation is a widely used technique to render any type of time-dependent data for a rapid navigation through the data. This gives a quick overview of the spatio-temperal behavior of the system. Our model renders atoms at their respective positions for one FPMD step at a time using spheres of different radii and colors differentiating their atomic types. Animation is supported in the ball representation (showing only atoms), ball-stick representation (showing inter-atomic bonds and their formation/breakage) and polyhedral forms. The bonds are color coded according to their lengths

whereas the polyhedra are color-coded according to the degree of the distortion from their ideal structure. In addition, animation is also coupled with rendering of several other spatio-characterization properties such as radial distribution function, coordination, displacement data, structural units and clusters.

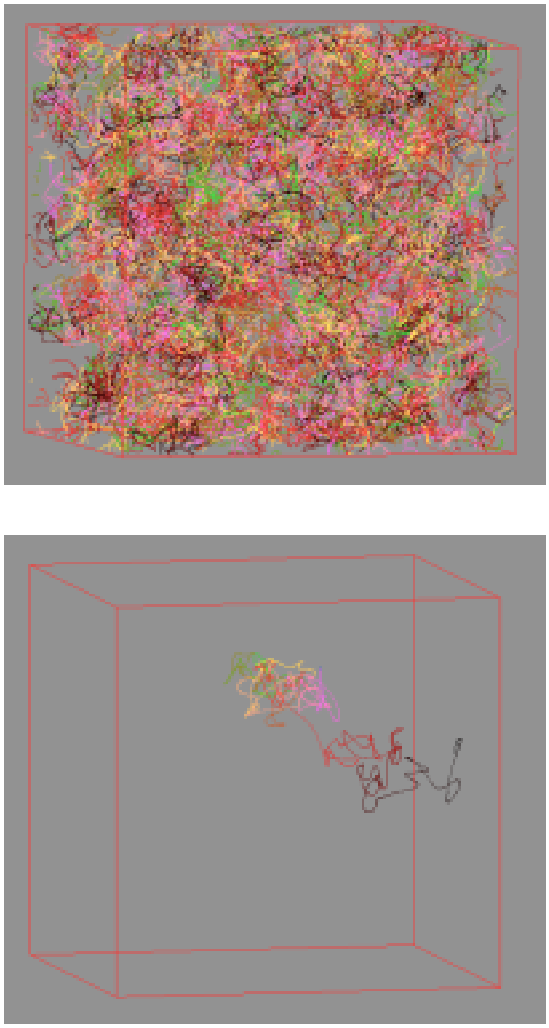

Figure 1: Pathlines of all 64 atoms (top) and the pathline of one selected atom (bottom) of the liquid MgO at 4000 K. The bottom clearly shows that the particle wanders in different regions as time elapses.

Pathlines

The complete trajectories of all or selected atoms are displayed as pathlines (Figure 1). The pathline technique is widely used to represent the flow of particles [Sch97]. As an atom moves within the supercell satisfying the periodic boundary conditions, its path is traced using a color-coded line. The pixel color at the position is varied according to the elapsed time. This allows us to easily visualize the history and extent of the atomic movement.

Color-mapped dimension

We propose a color-mapped dimension scheme to reduce the four-dimensional space-time data into two-dimensional representation. In this scheme, a given atomic position or displacement is mapped to a color with its red-component representing the x-coordinate, green-component representing the y-coordinate and blue-component representing the z-coordinate. The screen coordinates, horizontal and vertical screen axes, are used for representing simulation time step and the atoms, respectively. The pixels along some vertical line (parallel to the y-axis) correspond to different atoms at a given time whereas the pixels along some horizontal line (parallel to the x-axis) correspond to the positions or displacements of a particular atom as a function of time. The individual pixels displayed on the screen thus represent individual 4D space-time data points. Unlike the direct 3D particles' rendering, this does not suffer from any occlusion. However, there is no direct visual representation of the real 3D arrangement of atoms. Here, we place all Mg atoms in the lower half and O atoms in the upper half. The other way is to arrange the atoms in the form of 8-atoms unit cells, which are put together to form the supercell. For example, a combination of 2x2x2 unit cells makes up a 64-atoms supercell whereas 3x3x3 arrangement determines a 216-atom supercell.

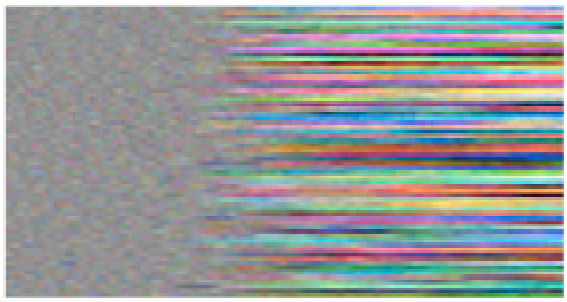

Figure 2: Color-mapped dimension representation of the atomic displacements relative to the perfect crystalline positions calculated over 3000 time steps (every 10 steps are skipped) across the solid-to-liquid phase transition in a 64-atom MgO system.

The purpose here is to visualize the differences between the consecutive atomic configurations or displacements corresponding to different phases and/or conditions. Figure 2 renders the atomic displacement data during the time period in which the solid-to-liquid phase transition takes place in MgO. We clearly see the contrast in the brightness of the pixels' colors between the left (solid phase) and right (liquid phase) portions of the image. The pixels' intensities and their variations for the liquid phase are much larger than those for the solid phase.

4.2 Local/Extracted Data Rendering

Radial distribution function

We compute the radial distribution functions (RDF), both partial and total, $g_{\alpha\beta}(r)$ and $g(r)$, and structure factor, $S(q)$ to examine the microstructures of the simulated system [Chel01, Allen87]. The RDF is the probability of finding another atom at a distance r from a specified atom. Computation of RDF is not straightforward due to the supercell structure and its periodicity, so the algorithm is presented here (Figure 3). The RDF information is often used to compute other structural properties, for instance, the positions of the first peak and the first minimum after the peak are used in the coordination and cluster analysis. Figure 4 shows the total RDF, $g(r)$, of the liquid MgO, which saturates to the unity after the first peak, indicating the absence of any long-range correlation among atoms – a characteristic feature of the liquid phase. On the other hand, the RDF of solid MgO shows several well-defined peaks. The structure factor (SF) is also calculated by taking the Fourier transform of RDF.

```
For each Simulation Step
 For i := 1 to n_a - 1
  For j := 1 to n_a
   dist := d(p_i(t), p_j(t))
   idx := dist/dr
   h_t(i)t(j)[idx]:= h_t(i)t(j)[idx]+1
  End
 End
End
v := a^3
pf := v/(4πn_t);
For i := 1 to n_s
 For j := 1 to n_s
  f := pf/n_i n_j
  For k := 1 to n_d
    ppcf_ijk :=f*h_ijk/(rh_k^2 dr);
  End
 End
End
For k := 1 to n_d
 pcf_k := 0.0;
 For i := 1 to n_s
  For j := 1 to n_s
     pcf_k :=pcf_k+ n_i n_j ppcf_ijk/n;
  End
 End
End
```

Figure 3: A pseudocode for the radial distribution function calculation. Here, n_a is the total number of atoms, n_i and n_j are the number of species `i` and `j`.

Coordination environment

The simplest and most common parameter, which characterizes the local structural information, is the coordination number. It indicates the average number of particles of species β around a particle of species α within a sphere of radius r. It is simply the integral over the corresponding radial distribution function [Chel01, Allen87]:

$$C_{\alpha\beta} = 4\pi\rho_\beta \int_0^{r_{min}} r^2 g_{\alpha\beta}(r)dr$$

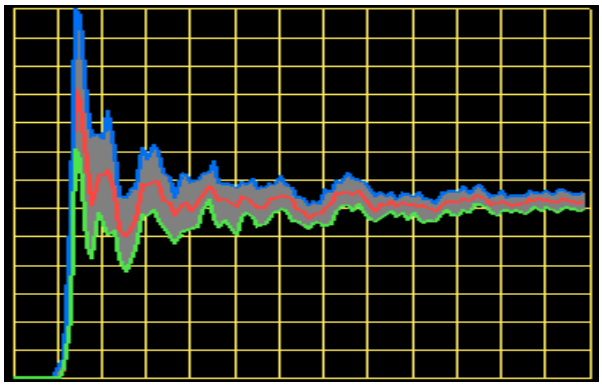

Figure 4: Plot of the RDF for the liquid MgO system as a function of distance, r (Blue: upper bound, Green: lower bound, Red: time averaged over 5000 steps)

Here, ρ is the number density and c_β is the concentration (N_β/N) of atoms of type β. Since we are interested only at the nearest neighbors, the cutoff is taken to be the first minimum (r_{min}) of the corresponding partial radial distribution function. We visualize the coordination as a function of space (per atom basis) in the form of simple bonding or polyhedral representation. The individual atoms or polyhedra are color-coded according to the calculated coordination numbers. As shown in Figure 5, the coordination environment is not uniform throughout the system. The coordination environment also gives substantial insight into the compositional disorder in the structure, i.e., the degree and nature of the mixing of homogeneous (like-atoms) and heterogeneous (unlike-atoms) bonding.

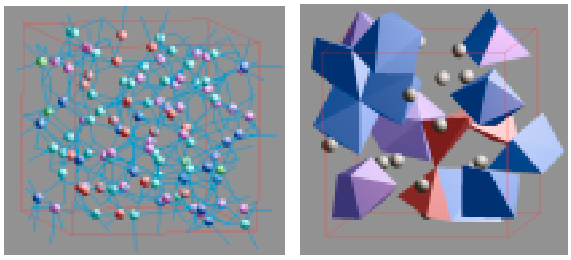

Figure 5: Mg-O coordination in the 216-atoms liquid MgO (left) and Si-O coordination in the 80-atoms liquid $MgSiO_3$ (right). Their space-time averaged values are 4.8 and 6.1, respectively. In MgO, 108 Mg atoms are shown with five green (coordination greater than 6), 16 blue (the six-fold coordination), 33 pink (five-fold coordination), 36 cyan (four-fold coordination) and 17 orange spheres (coordination smaller than 4). In $MgSiO_3$, the 16 Si-polyhedra are shown with 10 blue SiO_6 (octahedra), 3 purple SiO_7 units and 3 red SiO_5 and SiO_4 units. The polyhedra are constructed using the qhull algorithm [Barb96].

Cluster analysis

We adopt the following convention to obtain insight into the internal cluster structure: If we can traverse through a group of atoms following path from one atom to the another atom such that distance between any two consecutive atoms on the path are within a specified cutoff distance, then we say they are related in some fashion to form a cluster, which connects successive the nearest neighbor (NN) atoms [Jarvis73], as shown in Figure 6. For example, the relevant cutoff distance could be $r_{crystal}$ (crystalline bond-length), r_{peak} or r_{min} (distance to the first peak or the first minimum of RDF).

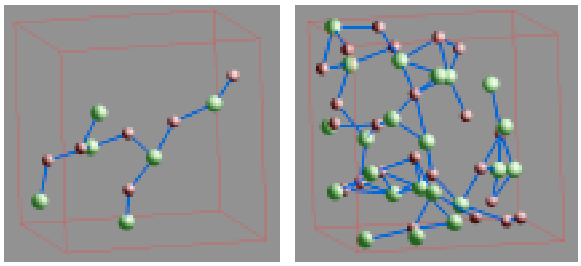

Figure 6: Nearest-neighbor (NN) clusters formed starting any atom in the cluster for different cutoff distances used: r_{peak} (*left*) and $r_{crystal}$ (*right*). Their size and shape characterize the structure at different length scales.

```
For i := 1 to n_a
 For j := i+1 to n_a
  For all a [] alisti
   If dist(i,a) < d_m mark_a := 1
  End
  For all a [] alist_j
   If d(j,a)< d_m and mark_a=1
     Then cn.add(a)
  End
  For all a [] cn
     For all b [] cn
      If a!=b and dist(a, b) < d_m
        Then (a,b):=BONDED
     End
  End
 End
End
```

Figure 6: Algorithm for common-neighbor (CN) analysis. Here, n_a is the total number of atoms. The minimun distance d_m is usually determined from RDF: the minimum after the first peak.

Common-neighbor (CN) analysis [Honey87, Blais84] is also used to analyze the cluster structures (Figure 7). It represents a way of decomposing the radial distribution function, g(r), according to the environment of the pairs. In this analysis, a pair is considered bonded if they are within the r_{min} distance of each other. For the purpose of cluster analysis, we represent the system as a graph $G = (V, E)$, where the atoms are the vertices, V, and the distance between two vertices, V_1 and V_2, is the weight for the edge, E, between those two atoms. The graph is stored in the form of an adjacency list. Given a vertex, V, only those vertices $V' \subset G$, which are within some maximum distance ($4r_{min}$) and hence contribute to the analysis, are kept in the adjacency list of V.

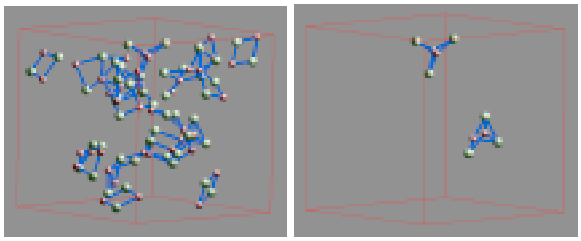

Figure 7: Common-neighbor (CN) clusters in the 216 atoms liquid MgO using r_{min} as the cutoff distance. Short chain-like structures for the pairs with two-CNs can be seen. Three-CNs which are always absent in the solid phase exist in the liquid phase. Their number, size and shape are found to vary greatly with time. The higher-order-CNs occasionally appears during the simulation.

Spheres of atomic movement

Visualization of the extent of the atomic movement or displacement during the simulation is useful to characterize the local and overall behavior of the dynamics of the given atomic system. We extract the several sets of atomic displacement data. They represent the differences of the atomic configuration at a given instant from the initial (perfect crystalline or some random) or previous or next configuration. The other relevant differences are those involving the farthest positions the atoms reach or the mean atomic positions during the whole simulation period. In each case, the magnitude of the displacement is represented by the size of the sphere located at each atomic position whereas the direction of the displacement is represented by a line segment pointing away from the surface of the sphere. Figure 8 shows the displacement patterns induced by point (vacancy) defects. The size of the spheres differs among different atomic species (shown by different colors) and, in the case of $MgSiO_3$, among the atoms of the same type (spheres of the same color). The lines are also oriented along various directions. The atomic displacement visualization thus implies that the defect effect is isotropic in MgO whereas it is anisotropic in $MgSiO_3$. We have also visualized the

liquid data to show that the diffusion process is anisotropic and non-uniform to different extents at different pressure and temperature conditions.

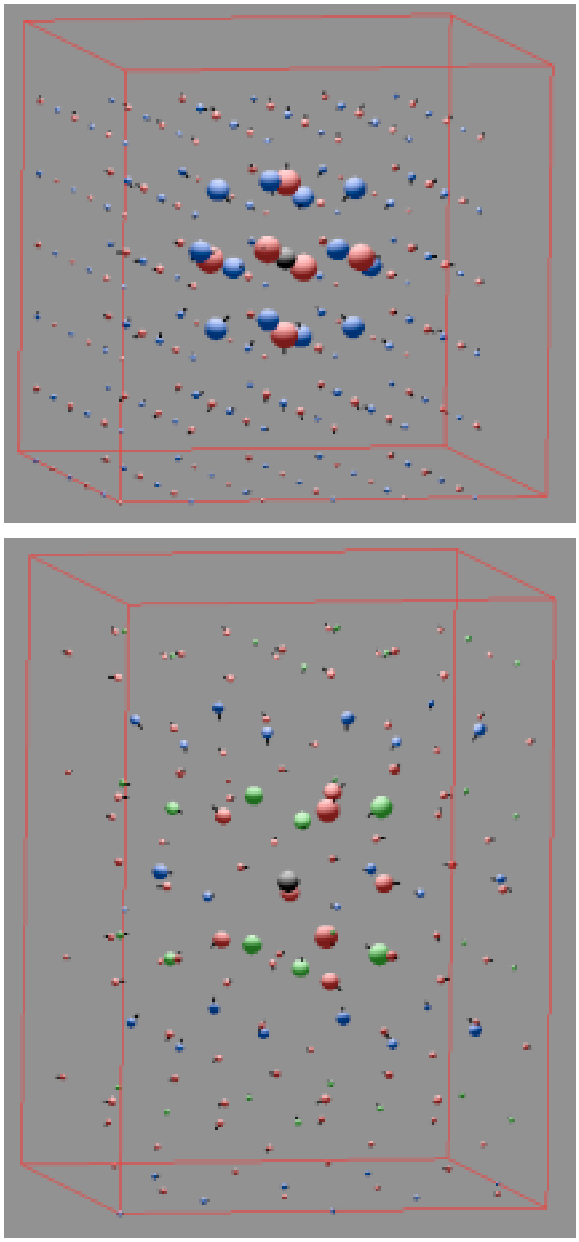

Figure 8: Visualization of atomic displacement data for defective 216-atom MgO (top) and 160-atom $MgSiO_3$ (bottom). The dark grey sphere indicates the vacancy site from where the Mg atom is removed in the both systems. Other spheres, blue, red and green, represent the extents of movement (or displacement relative to the perfect crystal positions) for Mg, O ant Si atoms, respectively.

5. IMPLEMENTATION

The proposed space-time multiresolution visualization scheme is implemented in a modular fashion (Figure 9) so it is easy to add additional modules whenever needed. In essence, the input configuration data (consisting of a given time series over 5000 steps of atomic 3D positions) are read into the memory. The data are used to generate additional data on the fly, which exploit the use of specific data-structures (e.g., adjacency lists) and dynamic memory allocation. Some datasets are generated dynamically and some are kept in the memory throughout the visualization process. For instance, for the Common Neighbor analysis, it is computationally as well as memory-wise prohibitive to compute all the clusters for all 5000 or so steps beforehand. Moreover, the clusters are dependent on the critical distance used for the analysis. The application lets the user interactively change the critical distance or the time step to study the cluster formation. On the other hand, the averaged RDF is computed once to obtain the r_{peak} and r_{min} values for their use later by other modules.

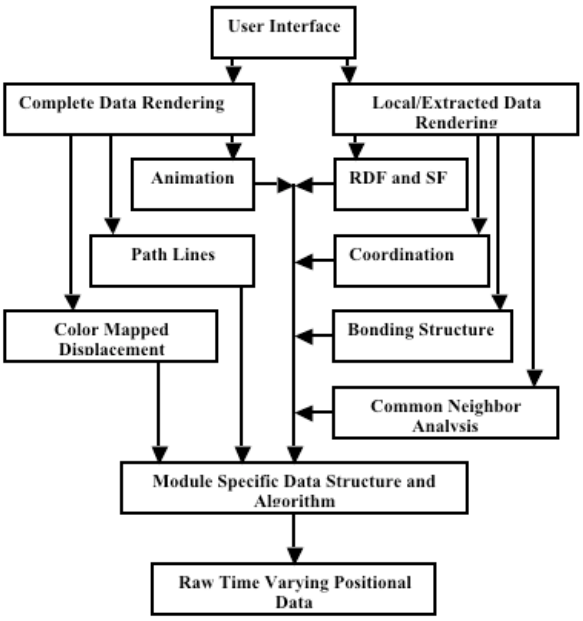

Figure 9: Various visualization modules and their relationship among each other.

Implementation is done using C, OpenGL, GLUT and GLUI. Performance measurements conducted on a Windows XP PC with 3.2 GHz Pentium IV processor, 1 GB RAM and 128 MB NVIDIA GeForce FX 5200 with 128 MB graphics card show that the interactive frame rates are achievable for all system sizes (64, 80, 160 and 216 atoms) considered in this study. The timings (which include the computation time and subsequent rendering time) are calculated for various modules for the 216-atoms system. The RDF module takes about 0.15 seconds per time step. The CN module takes 0.14, 0.18 and

0.25 seconds per time step for the cutoff distance equal to r_{peak}, $r_{crystal}$, and r_{min}, respectively. The NN-based cluster analysis module takes about 0.09 seconds per step. The time is about 0.02 seconds to draw the spheres of the atomic movement, and the time is even smaller for the execution of several other modules.

6. CONCLUSIONS

We have proposed an efficient visualization scheme to interactively explore the atomistic simulation data for the detailed spatio-temporal information for the structure and dynamics of a real material system. It adopts an application-based approach, which integrates several existing rendering and graph-theory techniques to fulfill the specific visualization needs imposed by the sophisticated first-principles materials modeling. In particular, it supports an interactive visualization of the original and on-the-fly-extracted data to gain insight into the atomic coordination, clustering and diffusion under different conditions and their variation with the time. In many cases, the physical relevance (atomic arrangement) needs to be rendered correctly, whereas, in other cases, only the information needs to be graphically rendered. There is still a lot to do with quantification and visualization of various interesting properties and processes, which are represented by simulation data. We plan to extend our approach by taking into account the additional data such as electron density. Interactivity and memory are expected to be the major issues in extension of the proposed scheme to the case of larger atomic systems.

7. ACKNOWLEDGMENTS

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